Relational Pooling for Graph Representations

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Abstract
This work generalizes graph neural networks (GNNs) beyond those based on the Weisfeiler-Lehman (WL) algorithm, graph Laplacians, and graph diffusion kernels. Our approach, denoted Relational Pooling (RP), draws from the theory of finite partial exchangeability to provide a framework with maximal representation power for graphs. RP can work with existing graph representation models, and somewhat counterintuitively, can make them even more powerful than the original WL isomorphism test. Additionally, RP is the first theoretically sound framework to use architectures like Recurrent Neural Networks and Convolutional Neural Networks for graph classification. RP also has graph kernels as a special case. We demonstrate improved performance of novel RP-based graph representations over current state-of-the-art methods on a number of tasks.

1. Introduction
Applications with relational graph data, such as molecule classification, social and biological network predictions, first order logic, and natural language understanding, require an effective representation of graph structures and their attributes. Representation learning for graph data has made tremendous progress in recent years. However, current schemes are unable to produce so-called most-powerful representations, which can provably distinguish all distinct graphs, up to graph isomorphisms. Consider the broad class of Weisfeiler-Lehman (WL) based Graph Neural Networks (WL-GNNs), for instance (Xu et al., 2019; Gilmer et al., 2017; Duvenaud et al., 2015; Kipf & Welling, 2016; Hamilton et al., 2017a; Velickovic et al., 2017; Monti et al., 2017; Ying et al., 2018). These cannot give distinct representations for graphs that cannot be distinguished by the standard WL isomorphism test (Cai et al., 1992; Xu et al., 2019). As graph neural networks are applied to increasingly more challenging problems, having a most-powerful framework for graph representation learning would be a key development in geometric deep learning (Bronstein et al., 2017).

In this work we introduce Relational Pooling (RP), a novel framework for graph neural networks that has provably maximal representation power for any graph input. While current approaches are mostly bottom-up, specified procedurally through transformations on graphs, RP takes a top-down approach, specifying an idealized most-powerful representation for graphs and then a framework to develop algorithms to approximate this ideal. The RP ideal can distinguish graphs not distinguishable by the WL isomorphism test, and, more surprisingly, we show that under the RP framework, practical algorithms based on WL-GNNs can be made to distinguish graphs not distinguishable by their corresponding WL-isomorphism test.

RP views relational learning as a pooling operation with partial invariances (graph isomorphism invariances), a framework inspired by the partial exchangeability of graph data (Aldous, 1981; Diaconis & Janson, 2008; Orbanz & Roy, 2015). RP differs from these earlier works by its focus on learning representations of finite but variable-size graphs. In particular, the RP function acts on a finite but arbitrary-sized graph $G$, which may be endowed with vertex or edge attributes, and outputs a single representation of the input, $\overline{f}(G)$, that is invariant to graph isomorphisms. Transductive and inductive models are both possible in RP, though in this paper, we will focus on inductive whole-graph embeddings to simplify our exposition.

Contributions. We make the following contributions:
1. We introduce Relational Pooling (RP), a novel framework for graph representation that can be combined with any existing neural network architecture, including ones not generally associated with graphs such as Recurrent Neural Networks (RNNs).
2. We prove that RP has maximal representation power for any graph input. We also show that WL-GNNs combined with RP (denoted RP-GNN) have more representation power than the WL test (or existing WL-GNNs). In our experiments, we classify graphs that cannot be distinguished by the standard WL test and an existing WL-GNN (Xu et al., 2019).
3. We introduce approximation approaches to make RP
2. Relational Pooling

Notation. Let $G = (V, E, X^{(v)}, X^{(e)})$ be an attributed graph, where $X^{(v)}$ is a $|V| \times d_v$ matrix representing node attributes and $X^{(e)}$ is a $|V| \times |V| \times d_e$ tensor representing edge attributes. W.l.o.g. the vertices are sequentially indexed: $V = \{1, \ldots, |V|\}$. A permutation is a bijective function on the vertex indices $\pi : V \rightarrow V$ and the set of all permutations $\Pi_{|V|}$ contains all such distinct mappings $\pi$. By definition, a permutation of $V$ does not alter the connectivity structure or attributes of a graph, thus we desire functions thereof to be permutation-invariant, or isomorphic-invariant.

Throughout this work we represent $G$ by two data structures: (1) a $|V| \times |V| \times (1 + d_e)$ tensor that combines $G$’s adjacency matrix with its edge attributes and (2) a $|V| \times d_v$ matrix representing node attributes $X^{(v)}$. The tensor is defined as $A_{v,u,i} = \mathbb{1}_{(v,u) \in E \times X^{(v)}}$ for $v,u \in \{1,2,\ldots,|V|\}$ where $\mathbb{1} \cdot \cdot \cdot$ denotes concatenation along the 3rd mode of the tensor, $\mathbb{1}_{(\cdot)}$ denotes the indicator function, and $X^{(v)}_{v,u}$ denotes the attributes of edge $(v,u)$ by a slight abuse of notation. Here, a (joint) permutation over the node indices is represented by $A_{\pi,v} \pi, \pi \pi, k = A_{i,j,k}$ and by $X^{(v)}_{\pi,v,\pi,\pi}$ defined as $(X^{(v)}_{\pi,v,\pi,\pi})_{i,j,l} = X^{(v)}_{\pi,v,\pi,\pi, l}$, $\forall i,j \in V$, $k \in \{1, \ldots, 1 + d_e\}$, $l \in \{1, \ldots, d_v\}$. Additional details and examples can be found in the Supplementary Material. Kearnes et al. (2016) shows a similar representation.

Joint RP. Inspired by joint exchangeability (Aldous, 1981; Diaconis & Janson, 2008; Orbanz & Roy, 2015), joint RP defines isomorphic-invariant functions over non-bipartite graphs, whether with directed or undirected edges, as

$$\bar{f}(G) = \frac{1}{|V|!} \sum_{\pi \in \Pi_{|V|}} \bar{f}(A_{\pi,v} \pi, X^{(v)}_{\pi,v}),$$

(1)

where $\bar{f}$ is an arbitrary (and possibly permutation-sensitive) function of the adjacency tensor and node attributes. We use the double-bar notation to denote a function that is invariant to any permutation $\pi$, following Murphy et al. (2019). Since equation 1 averages over all valid permutations, it is easy to see that $\bar{f}$ is an isomorphic-invariant function and can theoretically represent any such function $\overline{f}$ (consider $\bar{f} = \overline{f}$). Note that we can compose $\overline{f}$ with another function $\rho$ (outside the summation) to capture additional signal in the input (Murphy et al., 2019). This construction can give a maximally expressive graph representation (Theorem 2.1) that is intractable. In later sections we consider various neural network architectures for $\bar{f}$ and approaches to make the sum in equation 1 tractable.

Separate RP. In a bipartite graph (e.g., consumers x products) $V$ is composed of two disjoint sets $V^{(c)}$ and $V^{(v)}$, requiring separate exchangeability (Diaconis & Janson, 2008; Orbanz & Roy, 2015). Separate RP is defined for bipartite graphs to preserve separate invariance:

$$\bar{f}(G) = C \sum_{\pi^{(c)} \in \Pi_{|V^{(c)}|}} \sum_{\pi^{(v)} \in \Pi_{|V^{(v)}|}} \bar{f}(G_{\pi^{(c)}, \pi^{(v)})}$$

$$= C \sum_{\pi^{(c)} \in \Pi_{|V^{(c)}|}} \sum_{\pi^{(v)} \in \Pi_{|V^{(v)}|}} \bar{f}(A_{\pi^{(c)}, \pi^{(v)}, X^{(c,v)}, X^{(c,v)})},$$

(2)

where $C = (|V^{(c)}|! |V^{(v)}|!)^{-1}$, $\pi^{(c)}$ and $\pi^{(v)}$ are permutations of the rows and columns, respectively, and $X^{(c,v)}_{\pi^{(c)}, \pi^{(v)}}$ denote permutations of the attributes of $V^{(c)}$ and $V^{(v)}$, respectively. All of our results that apply to joint RP also apply to separate RP.

2.1. Representation Power of RP

Theorem 2.1. If node and edge attributes come from a finite set, then the representation $\bar{f}(G)$ in equation 1 is the most expressive representation of $G$, provided $\bar{f}$ is sufficiently expressive (e.g., a universal approximator).

All proofs are shown in the Supplementary Material. Theorem 2.1 shows that RP can be used to solve any graph-related regression or classification problem over finite graphs with finite attributes, including the problem of graph isomorphism (gives graph fingerprints that are unique between nonisomorphic graphs and shared between isomorphic graphs). The proof provides a key insight into the formulation of RP; a practitioner can focus on building highly expressive functions $\bar{f}$ that need not be isomorphic-invariant, and the RP summation assures that isomorphic-invariance is satisfied.

2.2. Neural Network Architectures

By allowing $\bar{f}$ to be permutation sensitive, RP allows the use of a wide range of neural network architectures, some of which we describe below.

RNNs, MLPs. A valid architecture to compute equation 1 is to vectorize the graph (concatenating node attributes with edge attributes) and learn $\bar{f}$ over the resulting sequence. The function $\bar{f}$ can be a recurrent neural network, like an LSTM (Hochreiter & Schmidhuber, 1997) or GRU (Cho et al., 2014), or a fixed-input function like a feedforward neural network (multilayer perceptron, MLP) with padding.
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if the sequences have different sizes. Concretely,
\[
\bar{f}(G) = \frac{1}{|V|!} \sum_{\pi \in \Pi_{|V|}} \bar{f}(\text{vec}(A_{\pi \pi}, X_{\pi}^{(\nu)}))
\]

Please refer to section A in the Supplementary Material for more details on the vec vectorization operator.

CNNs. Convolutional neural networks can also be directly applied over the tensor \( A_{\pi \pi} \) and combined with the node features \( X_{\pi}^{(\nu)} \), as in
\[
\bar{f}(G) = \frac{1}{|V|!} \sum_{\pi \in \Pi_{|V|}} \text{MLP}\left( \left[ \text{CNN}(A_{\pi \pi}) \times \text{MLP}(X_{\pi}^{(\nu)}) \right] \right)
\]

where \( \text{CNN} \) is a 2D convolutional neural network (LeCun et al., 1989; Krizhevsky et al., 2012) if there are no edge features and a 3D convolutional neural network (Ji et al., 2013) if there are edge features, \( \cdot \times \cdot \) is a concatenation of the representations, and \( \text{MLP} \) is a feedforward network (multilayer perceptron). The 3D CNN will often need to ensure that variable-sized graphs are mapped into the same sized representation. This can be achieved by multi-resolution 3D convolutions (Qi et al., 2016).

GNNs. The function \( \bar{f} \) can also be a graph neural network, a broad class of models which uses the graph \( G \) itself to define the computation graph. The models we consider follow a message-passing (Gilmer et al., 2017), or neighborhood aggregation, framework defined by the recursion
\[
h_u^{(l)} = \phi \left( h_u^{(l-1)}, J_P((h_v^{(l-1)})_{v \in N(u)}) \right),
\]

where \( \phi \) is a learnable function, \( J_P \) is a general (learnable) permutation-invariant function (Murphy et al., 2019), \( N(u) \) is the set of neighbors of \( u \in V \), and \( h_u^{(l)} \in \mathbb{R}^{d_l} \) is a vector describing the embedding of node \( u \) at layer \( 1 \leq l \leq L \) of the computation graph (\( h_u^{(0)} \) is defined as the \( u^{th} \) row of \( X^{(\nu)} \)). Under this framework, vertex embeddings can be used directly to predict vertex-level targets, or all vertex embeddings can be aggregated (via a learnable function) to form an embedding \( h_G \) used for graph-wide tasks. Xu et al. (2019) showed that these architectures can be at most as powerful as the Weisfeiler-Lehman (WL) algorithm for testing graph isomorphism (Weisfeiler & Lehman, 1968), which itself effectively follows a message-passing scheme. Accordingly, we will broadly refer to models following the message-passing scheme defined by equation 4 as WL-GNNs.

There are a number of variations of equation 4 in the literature. Among the earliest was Duvenaud et al. (2015), who proposed using embeddings from all layers \( l \in \{1, 2, \ldots, L\} \) for graph classification. Hamilton et al. (2017a) extended the framework to node classification and link prediction tasks, using the embedding at the last layer, while Xu et al. (2018) extend Hamilton et al. (2017a) by once again considering all embeddings at all layers for node and link prediction tasks. Other variations include attention (Velickovic et al., 2018) and similar improvements. An interesting perspective is that approximate spectral graph convolutions can be shown to yield models of this form (for instance, (Kipf & Welling, 2016)). Recently, Xu et al. (2019) propose an architecture called Graph Isomorphism Network (GIN) that they show to be as powerful as the WL test in representing isomorphic and nonisomorphic graphs with discrete attributes. More GNN models are discussed in section 3.

It might appear that there is no gain in using a WL-GNN for \( \bar{f} \) as it is invariant to \( \pi \), collapsing the sum of equation 1 into a single term. There are, however, two main advantages: (1) it allows WL-GNNs to be more powerful than the WL isomorphism test if we make \( \bar{f} \) permutation sensitive such as in the manner we describe below, and (2) it gives us a theoretically sound procedure to apply a WL-GNN over smaller random subgraphs of the original graph, rather than the entire graph, significantly speeding up GNNs. We will revisit (2) when we delve into tractability approaches to RP using \( k \)-ary dependencies.

Can a WL-GNN be more powerful than the WL test? WL-GNNs have a representation shortcoming that they inherit from the WL test (Arvind et al., 2017; Cai et al., 1992; Fürer, 2017). The node representation in a WL-GNN is incapable of encoding whether two nodes have the same neighbor or distinct neighbors with the same attributes. Consider a graph task where graphs represent molecules, with vertex attributes indicating the atom type and edges denoting the presence or absence of bonds. Here, the first WL-GNN layer is incapable of distinguishing that two (say) carbon atoms have a bond with the same carbon atom, or a bond to two distinct carbon atoms. As we move up the layers of the WL-GNN, node representations become node features in succeeding layers, and the hope is that eventually nodes get unique representations (up to isomorphisms), which would allow the WL-GNN to detect whether or not two nodes have the same neighbor based on the unique features of their neighbors.

However, if the WL-GNN does not have enough layers to guarantee unique node representations (up to isomorphisms) or if the graph has complex cycles, the WL-GNN will fail to correctly represent the graph and its nodes. To better understand this challenge, consider an extreme case illustrated with the two graphs in figure 1. These are cycle graphs with \( M = 11 \) nodes and skip links of different lengths around the circle \( R \in \{2, 3\} \) added to all pairs of vertices. These highly symmetric graphs are instances of circulant graphs and are well-known in the graph theory
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The two graphs are clearly distinct (nonisomorphic) but the WL algorithm—and thus any WL-GNN—is incapable of representing the nodes in the left graph distinctly from nodes in the right graph. Note that the vertex attributes are assumed to be initialized as \( h_{v_i}^{(0)} = c \), where \( c \) is some constant (usually 1, w.l.o.g.).

\[ M = 11, R = 2 \quad M = 11, R = 3 \]

Figure 1: Two nonisomorphic graphs deemed isomorphic by the WL test.

RP offers a flexible approach to make WL-GNN more expressive than its WL test. Let \( f \) be a WL-GNN that we make permutation sensitive by assigning each node an extra node attribute, such as a vertex identifier, that depends on \( \pi \). Intuitively, vertex identifiers help distinguish neighbors that otherwise appear identical and mitigate the problem illustrated by our ‘carbon atoms’ example above. In particular, the node in the \( v \)-th vertex in the permuted graph is assigned a one-hot encoding, which can be represented by augmenting the vertex attribute matrix to obtain

\[ X_{\pi}^{(v)} \otimes I_{|V|} \]

where \( I_{|V|} \) is a \(|V| \times |V|\) identity matrix and \([B \otimes C]\) concatenates the columns of matrices \( B \) and \( C \). RP-GNN is then given by

\[
\overline{f}(G) = \frac{1}{|V|!} \sum_{\pi \in \Pi_{|V|}} f \left( A_{\pi,\pi}, \left[ X_{\pi}^{(v)} \otimes I_{|V|} \right] \right)
\]

where the second holds since \( \overline{f} \) is an isomorphic-invariant GNN. Equation 5 is permutation-invariant while all nodes are guaranteed to have unique attributes. The following theorem proves that \( \overline{f}(G) \) in equation 5 is strictly more expressive than the original WL-GNN in that it can distinguish all nodes and graphs that WL-GNN can in addition to graphs that the original WL-GNN cannot. We provide further details on this formulation in the Supplementary Material.

**Theorem 2.2.** The RP-GNN in equation 5 is strictly more expressive than the original WL-GNN. Specifically, if \( \overline{f} \) is a GIN (Xu et al., 2019) and the graph has discrete attributes, its RP-GNN is more powerful than the WL test.

The power of RP-GNN in equation 5 comes at a heavy computational cost. Fortunately, there multiple ways to make equation 5 tractable while still retaining some of the power of RP-GNNs over standard GNNs. We leave tractability approaches that are common to other architectures to section 2.3. One approach that is specific to RP-GNN on attributed graphs adds just enough unique new ids to \( G \) to ensure that all node attributes in the graph are unique, reducing the number of permutations in equation 5. In a molecule, such as Hydroxyformaldehyde \( CH_2O_2 \), we only need to give extra ids to make atoms unique: \((C, 1), (H, 1), (H, 2), (O, 1), (O, 2)\). Now, only a total of \(1! \cdot 2! \cdot 2! = 4 \) permutations need to be considered in equation 5. An approximation, useful for unattributed graphs, assigns id \( i \mod m \) to node \( i \), where \( m = 1 \) is the original GNN and \( m = |V| \) is the most powerful RP-GNN.

### 2.3. RP Tractability

#### 2.3.1. Tractability through canonical orientations

By itself equation 1 is intractable, and calls for approximations of some sort. The most direct approach towards this is to compose a permutation-sensitive \( \overline{f} \) with a canonical orientation function that re-orders \( A \) such that

\[
\text{CANONICAL}(A, X^{(v)}) = \text{CANONICAL}(A_{\pi,\pi}, X_{\pi}^{(v)}), \quad \forall \pi \in \Pi_{|V|}.
\]

This causes the sum over all permutations to collapse to just an evaluation of \( \overline{f} \circ \text{CANONICAL} \). Essentially, this introduces a fixed component into the permutation invariant function \( \overline{f} \), with only the second stage learned from data. Note that this is not equivalent to the original problem as the CANONICAL function need not have learnable parameters (e.g. sorting by centrality scores). Such an approach is however only as useful as its canonical orientation, which if not strongly correlated with the objective function, can result in poor representations. Consider a scenario where we order nodes according to their degrees (breaking ties according to some rule) and suppose that the objective function is correlated with the vertex attributes but independent of vertex degrees. Effectively, this canonical orientation forms a single permutation of the vertex attribute matrix—likely differing from graph to graph—learning with which can result in poor task performance.

A more flexible approach collapses the set of all permutations into a much smaller set of equivalent permutations. We denote this approach poly-canonical orientation. Depth-First Search (DFS) and Breadth-First Search (BFS) node orderings are two examples of poly-canonical orientations. In a DFS, the nodes of the adjacency matrix/tensor \( A_{\pi,\pi} \) are ordered 1 to \( |V| \) according to the order they are visited by a DFS starting at \( \pi(1) \). Thus, if \( G \) is a length-three path and we consider permutation functions defined (elementwise) as \( \pi(1, 2, 3) = (1, 2, 3) \) and \( \pi'(1, 2, 3) = (1, 3, 2) \), our DFS or BFS would see respectively \( \decomp{(1, 2, 3)} \) and \( \decomp{(1, 3, 2)} \) (where vertices are numbered by permuted indices), start at \( \pi(1) = 1 \) and result in the same
left-to-right sorting for both permutations. If the graph is disconnected, the search starts at the first node of each connected component. Note that beyond the starting node, the search traversal order of neighbors of a node also depends on π. Learning canonical orders from data is a discrete optimization problem left for future work.

2.3.2. Tractability through π-SGD

The key approach to achieve tractable joint and separate RP is to sample random permutations during training. This approach offers the significant computational savings of a single canonical ordering while being considerably more flexible and robust, and avoids the need to learn a good canonical ordering for a given objective function.

For simplicity, we analyze the optimization with a single sampled permutation in a supervised graph classification setting, but this can be easily extended to sampling multiple permutations and unsupervised settings. Further, while we focus on joint invariance, the formulation is similar for separate invariance. Consider N training data examples \( D = \{(G(1), y(1)), \ldots, (G(N), y(N))\} \), where \( y(i) \in Y \) is the target output and graph \( G(i) \) its corresponding graph input. For a parameterized function \( f \) with parameters \( W \),

\[
\hat{f}(G(i); W) = \frac{1}{|V(i)|!} \sum_{\pi \in \Pi_{|V(i)|}} \bar{f}(A_{\pi}, \pi(i), X_{\pi}^{(v)}(i); W),
\]

our goal is to minimize the empirical loss

\[
\bar{L}(D; W) = \frac{1}{N} \sum_{i=1}^{N} L\left(y(i), \bar{f}(G(i); W)\right),
\]

where \( L \) is a convex loss function of \( \bar{f}(\cdot; \cdot) \) such as cross-entropy, negative log-likelihood, or square loss. Now, for each graph \( G(i) \) a random permutation \( s_i \) is sampled uniformly as \( s_i \sim \text{Uniform}(\Pi_{|V(i)|}) \), and we consider replacing the RP sum in equation 1 with the estimate

\[
\tilde{f}(G_{s_i, s_i}(i); W) = \bar{f}(A_{s_i, s_i}(i), X_{s_i}^{(v)}(i); W),
\]

where we have introduced the notation \( G_{s_i, s_i}(i) \) to denote a permutation of the corresponding tensor \( A \) and matrix \( X^{(v)} \). Note that, for separate invariance, we would write \( G_{s_i, s_i}(i) \) to indicate that one distinct permutation is sampled for each set of vertices. The estimator in equation 7 is unbiased:

\[
E_s[\tilde{f}(G_{s_i, s_i}(i); W)] = \bar{f}(G(i); W).
\]

Note however that when \( \tilde{f} \) is chained with a nonlinear loss \( L \), the composition is no longer unbiased:

\[
E_s[L(y(i), \tilde{f}(G_{s_i, s_i}(i); W))] \neq L(y(i), E_s[\tilde{f}(G_{s_i, s_i}(i); W)])
\].

Nevertheless, as we will soon justify, we follow Murphy et al. (2019) and use this estimate in our optimization, calling the resulting procedure \( \pi \)-SGD for RP:

**Definition 2.1** [\( \pi \)-SGD for RP] Let \( B_t = \{(G(1), y(1)), \ldots, (G(B), y(B))\} \) be a mini-batch i.i.d. sampled uniformly from the training data \( D \) at step \( t \). Consider the stochastic gradient descent update

\[
W_t = W_{t-1} - \eta_t Z_t,
\]

where \( Z_t = \frac{1}{B} \sum_{i=1}^{B} \nabla_{W_i} L\left(y(i), \tilde{f}(G_{s_i, s_i}(i); W_{t-1})\right) \) is the random gradient with the random permutations \( \{s_i\}_{i=1}^{B} \), (sampled independently \( s_i \sim \text{Uniform}(\Pi_{|V(i)|}) \) for all graphs \( G(i) \) in batch \( B_t \), and the learning rate is \( \eta_t \in (0, 1) \) s.t. \( \lim_{t \to \infty} \eta_t = 0 \), \( \sum_{t=1}^{\infty} \eta_t = \infty \), and \( \sum_{t=1}^{\infty} \eta_t^2 < \infty \).

Effectively, this is a Robbins-Monro stochastic approximation algorithm of gradient descent (Robbins & Monro, 1951; Bottou, 2012) and optimizes the following modified objective:

\[
\bar{f}(D; W) = \frac{1}{N} \sum_{i=1}^{N} E_{s_i} \left[L\left(y(i), \tilde{f}(G_{s_i, s_i}(i); W)\right)\right]
\]

\[
= \frac{1}{N} \sum_{i=1}^{N} \frac{1}{|V(i)|!} \sum_{\pi \in \Pi_{|V(i)|}} L\left(y(i), \tilde{f}(G_{\pi, \pi}(i); W)\right).
\]

Observe that the expectation over permutations is now outside the loss function (recall \( \bar{f}(G(i); W) \) in in equation 6 is an expectation). As in equation 6, the loss in equation 9 is also permutation-invariant, though we note that \( \pi \)-SGD, after a finite number of iterations, returns a \( \tilde{f}(G_{s_i, s_i}(i); W) \) sensitive to the random input permutations of \( G_{s_i, s_i}(i) \) presented to the algorithm. Further, unless the function \( \tilde{f} \) itself is permutation-invariant (\( \tilde{f} = \bar{f} \)), the optima of \( \bar{f} \) are different from those of the original objective function \( \bar{f} \). Instead, if \( L \) is convex in \( \bar{f}(\cdot; \cdot) \), \( \bar{f} \) is an upper bound to \( \tilde{f} \) via Jensen’s inequality, and minimizing this upper bound forms a tractable surrogate to the original RP objective in equation 6.

The next result draws on the \( \pi \)-SGD formulation of Murphy et al. (2019) showing the convergence properties of our stochastic optimization.

**Proposition 2.1.** [\( \pi \)-SGD Convergence (Murphy et al., 2019)] The optimization of \( \pi \)-SGD enjoys properties of almost sure convergence to the optimal \( W \) under similar conditions as SGD.

Given fixed point \( W^* \) of the \( \pi \)-SGD optimization and a new graph \( G \) at inference time, we may opt to exactly compute \( E_s[\tilde{f}(G_{s_i, \pi}(s_i); W^*)] = \tilde{f}(G; W^*) \) or estimate it with \( \frac{1}{m} \sum_{j=1}^{m} \tilde{f}(G_{s_j, \pi}(s_j); W^*) \) where \( s_1, \ldots, s_m \overset{i.i.d.}{\sim} \text{Uniform}(\Pi_{|V(i)|}) \).
2.3.3. Tractability through k-ary dependencies

In Murphy et al. (2019), the authors propose k-ary pooling wherein computational complexity is reduced from summing over all permutations of the input sequence to just subsequences of size k. In the context of statistical Markov Random Field models, exchangeability assumptions also provide a type of k-ary tractability (Nepier & Van den Broeck, 2014). Inspired by this, we propose k-ary Relational Pooling which operates on k-node induced subgraphs of \( G \). This corresponds to patches of size \( k \times k \times (d_e + 1) \) of \( \mathbf{A} \) and k rows of \( \mathbf{X}^{(v)} \). Formally, we define k-ary RP in joint RP by

\[
\bar{f}^{(k)}(G; \mathbf{W}) = \frac{1}{|V|!} \sum_{\pi \in \Pi_{|V|}} f^{(k)}(\mathbf{A}_{\pi \cdot \pi}, \mathbf{X}^{(v)}_{\pi}[:1:k,:]); \mathbf{W})
\]

(10)

where \( \mathbf{A}_{\cdot \cdot \cdot} \) denotes access to elements in the first, second, and third modes of \( \mathbf{A} \); \( a:b \) denotes selecting elements corresponding to indices from a to b inclusive; and “:” by itself denotes all elements along a mode. Thus, we permute the adjacency tensor and select edge-attribute fibers along the third mode from the upper left \( k \times k \times (d_e + 1) \) sub-tensor of \( \mathbf{A} \) as well as the vertex attributes from the first k rows of \( \mathbf{X}^{(v)} \). In practice, the relevant k-node induced subgraphs can be selected without permuting the entire tensor \( \mathbf{A} \) and matrix \( \mathbf{X}^{(v)} \). Separate RP needs two values \( k_1 \) and \( k_2 \), representing the number of vertices to be selected from each partite set as inputs, respectively.

An illustration of the joint k-ary RP is depicted in figure 2 over a 5-node undirected graph \( G \) with no vertex features. The graph is represented on the right with its original node indices shown. Its corresponding adjacency tensor \( \mathbf{A}_{\pi \cdot \pi} \) with permutation \( \pi(1, 2, 3, 4, 5) = (3, 4, 1, 2, 5) \) is shown on the left, depicted as a cube whose depth depicts the adjacency matrix (front matrix slice) and a one-dimensional edge feature (back matrix slice), and its first and second modes the five nodes in the graph. The first representation shows a shaded \( 3 \times 3 \times (1 + d_e) \) region where elements of \( \mathbf{A}_{\pi \cdot \pi} \) are considered as input to \( \bar{f}^{(3)} \) in a 3-ary joint RP. The highlighted nodes and edges on the right shows the corresponding 3-node induced subgraph in \( G \). More generally, we can make the following conclusion:

**Proposition 2.2.** The RP in equation 10 requires summing over all k-node induced subgraphs of \( G \), thus saving computation when \( k < |V| \), reducing the number of terms in the sum from \( |V|! \) to \( \frac{|V|!}{(|V| - k)!} \).

Even fewer computations are needed if \( \bar{f}^{(k)} \) is made permutation-invariant over its input (a k-node induced subgraph).

We now show that the set of k-ary RP functions is strictly more expressive than the set of \((k-1)\)-ary RP functions, \( 1 < k \leq |V| \).

**Proposition 2.3.** \( \bar{f}^{(k)} \) becomes strictly more expressive as \( k \) increases. That is, for any \( k \in \mathbb{N} \), define \( \mathcal{F}_k \) as the set of all permutation-invariant graph functions that can be represented by RP with k-ary dependencies. Then, \( \mathcal{F}_{k-1} \) is a proper subset of \( \mathcal{F}_k \) if \( k \leq |V| \). Thus, RP with k-ary dependencies can express any RP function with \((k-1)\)-ary dependencies, but the converse does not hold.

**Further computational savings.** Even over moderately-sized graphs, the number of k-node induced subgraphs can be very large. Here we propose approaches for further computational savings.

**Ignoring disconnected subgraphs:** In some applications, we may want to define \( \bar{f}(\mathbf{A}_{\pi \cdot \pi}, \ldots) = 0 \) for any permutation \( \pi \) whose first k nodes form a disconnected k-node induced subgraph in \( G \). In sparse graphs, the number of disconnected k-node induced subgraphs is orders of magnitude larger than the number of connected subgraphs, mak-
ing this \( \bar{f} \) assumption bear out tremendous computational benefits.

**Use of \( \pi \)-SGD:** Here, we can combine the \( k \)-ary approximation with other computational savings such as \( \pi \)-SGD and poly-canonical orientations. For instance, a forward pass can consist of sampling a random starting vertex, performing a BFS orientation of \( \tilde{A} \), and selecting the left corner \( k \times k \times (d_v + 1) \) block of \( \tilde{A} \) (which is a connected induced subgraph by virtue of the BFS). The BFS does not need to be run over the entire graph. This approach, however, will be biased and unable to consider all possible connected induced subgraphs. An unbiased estimate over connected induced subgraphs can be achieved with the MCMC finite-sample unbiased estimator of Teixeira et al. (2018).

**Graph kernels as special cases of \( k \)-ary RP.** Graph kernels of Yanardag & Vishwanathan (2015) are special cases of \( k \)-ary RP where we assume node and edge attributes are discrete and we hand-pick the \( \bar{f}(A_{\pi,\pi}[1:k,1:k,:),X_{\pi}^{(0)}[1:k,:]) \) as a one-hot encoding over the input \( k \)-node subgraph \( A_{\pi,\pi}[1:k,1:k,:) \) with attributes \( X_{\pi}^{(0)}[1:k,:]. \) The sum over all permutations will be \( k! \) times the frequency of \( k \)-node subgraphs, which is the basis of Yanardag & Vishwanathan (2015).

### 3. Related Work

Graph Neural Networks (GNNs) and Graph Convolutional Networks (GCNs) form an increasingly popular class of methods (Xu et al., 2019; Gilmer et al., 2017; Bruna et al., 2013; Niepert et al., 2016; Defferrard et al., 2016; Duvenaud et al., 2015; Atwood & Towsley, 2016; Kipf & Welling, 2016; Hamilton et al., 2017a; Lee et al., 2018; Veličković et al., 2017; Monti et al., 2017; Meng et al., 2018; Xu et al., 2018; Scarselli et al., 2009). Applications include chemistry, where we may represent a dataset of molecules as a collection of undirected graphs in which vertices represent atoms, edges represent bonds, attributes on edges and/or vertices represent such characteristics as bonding type and charge, and we predict chemical properties like toxicity or photovoltaic efficiency (Gilmer et al., 2017; Duvenaud et al., 2015; Lee et al., 2018; Wu et al., 2018; Sanchez-Lengeling & Aspuru-Guzik, 2018); document classification wherein a network of documents has vertices representing documents, edges representing citations or hyperlinks, and vertex attributes representing document text (Hamilton et al., 2017b); and many others (cf. Battaglia et al., 2018).

Recently, Xu et al. (2019) shows that such methods are at most as powerful as the standard Weisfeiler-Lehman algorithm (also known as color refinement or naive vertex classification (Arvind et al., 2017; Fürer, 2017)) for graph isomorphism testing (Weisfeiler & Lehman, 1968) which fails to distinguish between certain classes of graphs such as regular graphs with the same number of nodes, edges, and degrees (Arvind et al., 2017; Cai et al., 1992; Fürer, 2017). In section 4, we demonstrate this phenomenon and provide empirical evidence that RP can correct some of these shortcomings of WL-GNNs. Higher-order \((k-\text{th order})\) versions of the Weisfeiler-Lehman isomorphism test WL[k] do exist (Fürer, 2017), where for WL[2] the algorithm operates on ordered pairs of vertices rather than just vertices. Except for Meng et al. (2018), which introduces a WL[k]-type graph representation to successfully predict high-order dynamics in temporal graphs, all existing GNNs are based on WL[1]-type isomorphism tests. Higher-order WL tests may be able to give better \( \bar{f} \) functions but are outside the scope of this work. We have provided a most-powerful representation and demonstrated that it is more expressive than these WL[1] procedures.

Closer to the RP approach, Montavon et al. (2012) discusses models that use a sorting scheme of a Coulomb matrix for molecules with limited random permutations. However, RP provides a significantly more comprehensive and general framework (with theoretical analysis). Orthogonally, CNNs have been used with graph kernels (Nikolentzos et al., 2018) and some GCNs can be seen as CNNs applied to single canonical orderings (Niepert et al., 2016; Defferrard et al., 2016); RP provides a framework for stochastic optimization over all orderings and over poly-canonical orderings.

In parallel, Bloem-Reddy & Teh (2019) generalizes functions that are invariant to graph permutations to those that are invariant to general group actions, discussing the connections to exchangeable probability distributions (De Finetti, 1937; Aldous, 1981; Diaconis & Janson, 2008). Their theoretical analysis uses a checkerboard function (Orbanz & Roy, 2015) to provide a canonical orientation of the adjacency matrix — that is, a way to map pairs of nonisomorphic graphs to different representations and pairs of isomorphic graphs to the same representation. The translation of these insights into practical algorithms is not yet clear. The canonical orientation cannot be computed in polynomial time unless the graph isomorphism problem can be solved in polynomial time — that is, the use of the left-order canonical orientation algorithm of Gharamani & Griffiths (2006) proposed by Bloem-Reddy & Teh (2019) will sometimes fail to give a proper canonical orientation for some classes of graphs. Using a single canonical orientation — rather than, say, poly-canonical orientations — also has the same drawbacks as using a single canonical orientation for permutation-invariance over sequence inputs, see the example in Murphy et al. (2019).

### 4. Experiments

In this section we focus on two types of experiments. The first shows that RP-GNN is more expressive than WL-
GIN. The second describes how \( k \)-ary tractability and \( \pi \)-SGD in the RP framework can make WL-GNN more scalable.

### 4.1. Testing RP-GNN vs WL-GNN

In this section we generalize and perform experiments over the class of graphs represented in figure 1. Here we show that WL-GNNs are necessarily limited in their power to represent the graph structures, and we show how RP can be used to ameliorate or even overcome this limitation. Our experiments compare the RP-GNN of equation 5 using the Graph Isomorphism Network (GIN) architecture (Xu et al., 2019) as \( f \) against the original GIN architecture. We choose GIN because it is arguably the most expressive WL-GNN architecture.

We now generalize the construction of the 4-regular graphs shown in figure 1. Here, the “skip length” \( R \) structural attribute effectively defines an isomorphism class in the sense that predicting \( R \) is tantamount to classifying a graph into its isomorphism class. We are interested in predicting \( R \) as an assessment of RP’s ability to exploit graph structure. Note we do not claim to attempt to solve the graph isomorphism problem since our approach will use approximate learning (\( \pi \)-SGD) for RP).

**Definition 4.1:** [Circulant Skip Links (CSL) graphs] Consider 4-regular undirected graphs \( G_{\text{skip}}(M, R) \) such that the \( M \) vertices form a cycle graph (circle) and each vertex is connected to those vertices exactly \( R \) hops away around the circle. Let \( R \) and \( M \) be co-prime natural numbers\(^1\) such that \( R < M - 1 \). Recursively define the sequence \( s_1 = 0, s_{i+1} = (s_i + R) \mod M \). We denote by \( G_{\text{skip}}(M, R) \) the undirected graph whose vertices are \( \{0, 1, \ldots, M - 1\} \) and whose edges are consecutive elements in the sequence: \( (s_i, s_{i+1}) \in E \) for any \( i \in \mathbb{N} \).

Note that there exist \( R_1 \neq R_2 \) such that \( G_{\text{skip}}(M, R_1) \) and \( G_{\text{skip}}(M, R_2) \) are isomorphic, but we are more interested in the cases when they are nonisomorphic.

**RP-GIN** Since WL-GNNs are expected to fail at this task, we will define an RP-GNN that we expect to succeed. GIN (Xu et al., 2019) follows the recursive update of equation 4 over \( L \) layers, replacing JP with a summation and defining \( \phi \) as a function that sums its arguments and feeds them through a multilayer perceptron:

\[
h_u^{(l)} = \text{MLP}^{(l)} \left( (1 + \epsilon^{(l)}) h_u^{(l-1)} + \sum_{v \in \mathcal{N}(u)} h_v^{(l-1)} \right),
\]

for \( l = 1, \ldots, L \), where \( \{\epsilon^{(l)}\}_{l=1}^L \) can be treated as hyper-parameters or learned parameters. This recursion yields

\(^1\)Two numbers are co-primes if they share no common factors other than one.
This domain provides challenging tasks on which to evaluate RP, while in other applications, different GNN models often achieve similar performance (Xu et al., 2019; Shchur et al., 2018). We leveraged the MoleculeNet project (Wu et al., 2018), which collects chemical datasets and reports the performance of various models, for choosing our datasets. We chose three on which graph-based models achieved superior performance\(^2\): HIV, MUV (Rohrer & Baumann, 2009), and Tox21 (Mayr et al., 2016; Huang et al., 2016).

These datasets contain measurements on a molecule’s biological activity, ability to inhibit HIV, and qualitative toxicity measurements for the MUV, HIV, and Tox21 datasets, respectively. All response variables are discrete, resulting in classification tasks. The datasets were processed with DeepChem (Ramsundar et al., 2019) and we evaluate all models with ROC-AUC following the MoleculeNet project. All compounds across all datasets are represented by graphs with 75-dimensional vertex (atom) attributes and 14-dimensional edge attributes. An example of a vertex attribute is a one-hot encoding of atom type. The number of molecules and tasks in each dataset is shown in Table 3 in the Supplementary Material.

We evaluate models using RP against the best performing baseline, as reported by MoleculeNet, a model based on the Graph Convolution proposed in Duvenaud et al. (2015) and implemented in DeepChem (by Altae-Tran et al. (2017)). We also implemented GIN (Xu et al., 2019) but it was unable to outperform the molecule-specialized model of Duvenaud et al. (2015); for instance, this model trains a different weight matrix \(W^{(i)}_k\) for each possible degree \(k\) of a vertex, which would be infeasible in other applications (\(\phi\) in equation 4 is replaced with \(\phi_x\)). We re-trained the DeepChem models using the same number of epochs as the other models we consider to make them more comparable. That being said, many models reached optimal performance before the last epoch; we use the model with best validation-set performance from training for test-set prediction. Our code is available on GitHub\(^3\), and the model architecture, hyperparameters, and training details are discussed in the Supplementary Material.

| model               | HIV       | MUV       | Tox21      |
|---------------------|-----------|-----------|------------|
| Duvenaud et al.     | 0.812 (0.014) | 0.807 (0.016) | 0.794 (0.010) |
| RP-Duvenaud         | 0.832 (0.013) | 0.809 (0.025) | 0.799 (0.006) |

Table 1: Comparison of RP-GNN and GNN on three molecule datasets. The GNN model is based on Duvenaud et al. (2015) and the RP-GNN uses this GNN as \(f\). We report the mean ROC-AUC and standard deviations in parentheses across random train/val/test splits. The RP-GNN is trained with \(\pi\)-SGD with 20 inference-time permutations sampled with \(\pi\)-SGD and sample 20 permutations at inference time. To quantify variability, we train over 20 random folds for Tox21 and HIV and 10 folds for MUV (please see the Supplementary Material for additional details).

The results shown in Table 1 suggest that RP-Duvenaud is more powerful than the baseline on the HIV task and similar in performance on the other two. While we bear in mind the over-confidence in the variability estimates (c.f. Bengio & Grandvalet (2004)), this experiment does support our theory regarding the power of RP-GNNs.

\(k\)-ary RP-GNN experiments Next we address two complementary questions related to the \(k\)-ary dependency models – evaluating \(\hat{f}\) on \(k\)-node induced subgraphs – discussed in section 2.3.3. First, proposition 2.3 shows that expressive power is lost as \(k\) decreases. Second, the computational complexity should also decrease with \(k\). To empirically evaluate these, we implement \(k\)-ary RP with \(\hat{f}\) represented by the model of Duvenaud et al. (2015) in equation 10. We consider \(k = 10, 20, 30, 40, 50\), where the percentage of molecules with greater than \(k\) atoms are: 98.18\%, 63.71\%, 22.30\%, 7.71\%, 3.59\% for HIV, 99.93\%, 75.33\%, 12.30\%, 0.03\%, 0.00\% for MUV, and 78.07\%, 33.63\%, 10.39\%, 3.90\%, 1.97\% for Tox21.

The \(k\)-ary RP-GNN is trained using \(\pi\)-SGD, and evaluated using five random train/validation/test splits. Results are shown in Table 2 and figures 4, 5, and 6 in the Supplementary Material. With the Tox21 dataset, we see a steady improvement in performance and computation as \(k\) increases but the benefits level off around \(k = 30\). In particular, \(k\)-ary with \(k = 10\) is 25\% faster than the baseline with AUC 0.687 (±0.005 std), with \(k = 20\) being 10\% faster with AUC 0.755 (±0.003 std), and \(k = 30\) about 5\% faster with AUC 0.775 (±0.011 std), where (±x) indicates the standard deviation over 5 bootstrapped runs (see also figure 4). For the other two datasets, both predictive performance and computation do not vary significantly with \(k\). Overall, the molecules are quite small, thus we do not expect to observe dramatic large computational gains with smaller \(k\).

RP with CNNs and RNNs. We now explore 20-ary RP with \(\hat{f}\) as a CNN, learned with \(\pi\)-SGD. At each forward

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\(^2\)Latest results available at [http://moleculenet.ai/latest-results](http://moleculenet.ai/latest-results), accessed December 2018

\(^3\)https://github.com/PurdueMINDS/RelationalPooling
In this work, we proposed a framework, Relational Pooling (RP), for graph classification and regression tasks. Our RP framework is shown to give ideal most powerful, though intractable, graph representations. We then propose a number of approaches to tractably approximate this ideal. We show, both theoretically and empirically, that RP allows a WL-GNN to be more expressive than its WL test, and permits neural network architectures like RNNs and CNNs to be brought to such problems. In our experiments, we evaluate these on a number of datasets, showing how our framework can be used to improve properties of state-of-the-art methods. Among future directions for theoretical study is to better understand the representational power of our tractable approaches, as well as the trade-offs that they involve.

5. Conclusions

In this work, we proposed a framework, Relational Pooling (RP), for graph classification and regression tasks. Our RP framework is shown to give ideal most powerful, though intractable, graph representations. We then propose a number of approaches to tractably approximate this ideal. We show, both theoretically and empirically, that RP allows

| $k$ | HIV | MUV | Tox21 |
|-----|-----|-----|-------|
| 60  | 0.818 (0.022) | 0.768 (0.014) | 0.778 (0.007) |
| 40  | 0.807 (0.025) | 0.776 (0.032) | 0.783 (0.007) |
| 30  | 0.829 (0.024) | 0.776 (0.030) | 0.775 (0.011) |
| 20  | 0.813 (0.017) | 0.777 (0.041) | 0.755 (0.003) |
| 10  | 0.812 (0.035) | 0.773 (0.045) | 0.687 (0.005) |
| CNN-DFS | 0.542 (0.004) | 0.601 (0.042) | 0.597 (0.006) |
| RNN-DFS | 0.627 (0.007) | 0.648 (0.014) | 0.748 (0.055) |

We also consider RP with an RNN as $\tilde{f}$ learned with $\pi$-SGD, again starting with a DFS to yield a $|V| \times |V| \times 14$ subtensor. For $\tilde{f}$, we treat the edge features of a given vertex as a sequence: for vertex $v$, we apply an LSTM to the sequence $(h_{A,v}, \ldots, h_{A,v})$ and extract the long-term state. We also take the vertex attributes and pass them through an MLP. The long-term state and output of the MLP are concatenated, ultimately forming a representation for every vertex (and its neighborhood) which we view as a second sequence. We apply a second LSTM and again extract the long-term state, which can be denoted $h_G$, the embedding of the graph. Last, $h_G$ is forwarded through an MLP yielding a class prediction. Twenty permutations were sampled at inference time. Variability was quantified with 5 random train/val/test splits for both neural network based models. Interestingly, Table 2 shows that the RP-RNN approach performs reasonably well in the Tox21 dataset, while underperforming in other datasets. Future work is needed to determine those tasks for which the RNN and CNN approaches are better suited.

Acknowledgments

This work was sponsored in part by the ARO, under the U.S. Army Research Laboratory contract number W911NF-09-2-0053, the Purdue Integrative Data Science Initiative and the Purdue Research foundation, the DOD through SERC under contract number HQ0034-13-D-0004 RT #206, and the National Science Foundation under contract numbers IIS-1816499 and DMS-1812197.

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Supplementary Material of Relational Pooling

A. Tensor Representation and vec Operation on Graphs

We briefly provide a concrete example of the representation of graphs and the operation vec(G). Consider a graph with three vertices, one edge attribute at each edge, and two vertex attributes at each vertex. The connectivity structure and edge attributes are represented by the 3 × 3 × 2 adjacency tensor \( \mathbf{A} \) where \( A_{i,j,k} \) denotes the value of the graph’s adjacency matrix and \( A_{i,j,k} \) denotes the value of the additional edge attribute, \( i, j \in V = \{1, 2, 3\} \).

\[
\begin{array}{cccc}
A_{(1,1,1)} & A_{(1,1,2)} & A_{(1,2,2)} & A_{(1,3,2)} \\
A_{(1,2,1)} & A_{(1,2,2)} & A_{(2,2,2)} & A_{(2,3,2)} \\
A_{(2,2,1)} & A_{(2,3,1)} & A_{(2,3,2)} & A_{(3,3,2)} \\
A_{(3,3,1)} & A_{(3,3,2)} & A_{(3,3,2)} & A_{(3,3,1)} \\
\end{array}
\]

Observe that the possibility of attributed self-loops is contemplated but this representation is applicable both to graphs that have self-loops and those that do not. The vertex attributes are represented in a matrix

\[
X^{(v)} = \begin{pmatrix}
X_{1,1} & X_{1,2} \\
X_{2,1} & X_{2,2} \\
X_{3,1} & X_{3,2}
\end{pmatrix}
\]

A simple vec operation is shown below. The modeler is free to make modifications such as applying an MLP to the vertex attributes before concatenating with the edge attributes. Representing \( G \) by \( \mathbf{A} \) and \( X^{(v)} \),

\[
\text{vec}(G) = (A_{(1,1,1)}, A_{(1,1,2)}, A_{(1,2,1)}, A_{(1,2,2)}, A_{(1,3,1)}, A_{(1,3,2)}, A_{(1,3,2)}, A_{(2,2,1)}, A_{(2,3,2)}, A_{(2,3,3)}, A_{(2,3,2)}, A_{(3,1,1)}, A_{(3,1,2)}, A_{(3,2,1)}, A_{(3,2,2)}, A_{(3,3,1)}, A_{(3,3,2)}, X_{3,1}, X_{3,2})
\]

Starting with the first vertex, each edge attribute (including the edge indicator) is listed, then the vertex attributes are added before doing the same with subsequent vertices. The vectorization method for \( k \)-ary type models is similar, except that we apply vec on induced subgraphs of size \( k \).

B. More on Unique Identifiers and WL-GNN Models

Here we elaborate on the addition of unique identifiers to graphs and implications for WL-GNN models. For simplicity, we consider undirected graphs with vertex attributes but no edge attributes, allowing us to simplify our notation to an adjacency matrix \( \mathbf{A} \) and vertex attribute matrix \( \mathbf{X} \). We also consider an oversimplified model with just one GNN layer \( (L = 1) \), the following aggregation scheme

\[
h_u = x_u + \sum_{v \in N(u)} x_v, \quad \forall u \in V;
\]

and the following read-out function to yield a graph representation

\[
h_G = \sum_{v \in V} h_v.
\]

This can be expressed as \( h_G = \mathbf{1}^T (\mathbf{A} + I_{|V|}) \mathbf{X} \) for adjacency matrix \( \mathbf{A} \), vertex attribute matrix \( \mathbf{X} \), identity matrix \( I_{|V|} \), and where \( \mathbf{1}^T \) is a row vector of ones.

For instance, we may observe the following graph with endowed vertex attributes. The numbers indicate vertex features, not labels.

\[
\begin{array}{c}
6 \\
5 \\
2 \\
1
\end{array}
\]

We can represent this with an adjacency matrix and vertex attribute matrix as

\[
\mathbf{A} = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 \\
1 & 1 & 1 & 0
\end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix}
0 \\
2 \\
1 \\
5
\end{pmatrix}
\]

Here, \( \mathbf{1}^T (\mathbf{A} + I_{|V|}) \mathbf{X} = 41 \). Equivalently, we might have chosen to represent this graph as

\[
\mathbf{A}_{\pi, \pi} = \begin{pmatrix}
0 & 0 & 1 \\
1 & 1 & 1 \\
0 & 1 & 1
\end{pmatrix}, \quad \mathbf{X}_\pi = \begin{pmatrix}
0 \\
2 \\
1
\end{pmatrix}
\]

Here we swapped the third and fourth column of \( \mathbf{X} \) and the third and fourth row and column of \( \mathbf{A} \). Yet again, \( \mathbf{1}^T (\mathbf{A}_{\pi, \pi} + I_{|V|}) \mathbf{X}_\pi = 41 \), as desired for isomorphic-invariant functions. We have chosen to assign scalar vertex attributes, but the invariance to permutation holds for vector vertex attributes.
Now, we propose assigning unique one-hot IDs after constructing the adjacency matrix, which corresponds to the following representations

\[ A = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \quad [X \otimes I_{|V|}] = \begin{pmatrix} 6 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]

\[ A_{\pi,\pi} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \quad [X_{\pi} \otimes I_{|V|}] = \begin{pmatrix} 6 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \]

(recall that \([\cdot \otimes \cdot]\) denotes concatenation). Note that we effectively assign identifiers after constructing \(A\) and \(X\) (and similarly for \(A_{\pi,\pi}, X_{\pi}\)), so that the latter four columns of \([X \otimes I_{|V|}]\) and \([X_{\pi} \otimes I_{|V|}]\) are the same.

Now, \(1^T(A + I_{|V|}) [X \otimes I_{|V|}] = (41, 2, 3, 4, 3, 3)\) yet \(1^T(A_{\pi,\pi} + I_{|V|}) [X_{\pi} \otimes I_{|V|}] = (41, 2, 3, 4, 3)\). This permutation sensitivity in the presence of unique IDs holds for more general WL-GNNs and not just the one considered here. Often \(h_G\) is fed forward through a linear or more complex layer to obtain the final graph-level prediction and this layer is usually permutation sensitive. Thus, we apply RP to GNNs with unique IDs to guarantee permutation invariance; meanwhile, the intuition for using unique IDs is to better distinguish vertices and thus create a more powerful representation for the graph.

### B.1. An alternative approach to RP-GNN models

Next we present an equivalent but alternative representation of RP-GNN models (equation 5) that may be simpler to implement in practice and provide an example. In the previous section, we described permuting the adjacency tensor and matrix of endowed vertex attributes, leaving the matrix of identifiers unchanged. Alternatively, with \(\bar{f}\) modeled as an isomorphic-invariant Graph Neural Network, one may leave the former two unchanged and instead permute the matrix of identifiers. Thus, the alternative model becomes

\[
\bar{f}(G) = \frac{1}{|V|} \sum_{\pi \in \Pi_{|V|}} \bar{f}(A_{\pi,\pi}, X_{\pi}^{(v)}),
\]

where \((I_{|V|})_{\pi}\) denotes a permutation of the rows of the identity matrix. The more tractable version discussed previously of assigning a one-hot encoding of the id \(i\) mod \(n\) to node \(i \in V\), for some \(n \in \{1, 2, \ldots, |V|\}\) is still applicable. In this case, we replace \((I_{|V|})_{\pi}\) with a \(|V| \times m\) matrix of \(m\)-bit one-hot identifiers, appropriately permuted by \(\pi\).

For example, consider again the graph defined by adjacency matrix \(A\) and vertex features \(X\) given above. To evaluate \(\bar{f}(A_{\pi,\pi}, X_{\pi})\) when the permutation is given by \(\pi(1, 2, 3, 4) = (2, 1, 3, 4)\), we could forward

\[
A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \quad [X \otimes (I_{|V|})_{\pi}] = \begin{pmatrix} 6 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 2 & 1 & 0 & 0 \end{pmatrix} \]

through our model of \(\bar{f}\). Previously the first row of \([X \otimes I_{|V|}]\) was \((6, 1, 0, 0, 0)\) whereas after permutation by \(\pi\) it became \((6, 0, 1, 0, 0)\), and so on. Both formulations discussed in this section were used in our experiments.

### Proof of Theorem 2.1

**Proof.** Let \(\Omega\) be a finite set of graphs \(G = (A, X^{(v)})\) that includes all graph topologies of finite size, as well as the associated vertex and edge attributes from a finite set. Note that isomorphic graphs \(G\) and \(G_{\pi,\pi}\) are considered distinct elements in \(\Omega\); observe that we are using the notation introduced in equation 2 and 7 where \(G_{\pi,\pi}\) denotes a permutation of \(A\) and \(X^{(v)}\). If \(G = (V, E, X^{(v)}, X^{(e)}) = (A, X^{(v)})\), let \(\mathcal{G}(G) = \{G_{\pi,\pi}, X^{(v)}_{\pi} : \pi \in \Pi_{|V|}\}\) denote the set of graphs that are isomorphic to \(G\) and have the same vertex and edge attribute matrices if the vertices were aligned. Consider a classification/prediction task where \(G \in \Omega\) is assigned a target value \(t(G)\) from a collection of \(|\Omega|\) possible values, such that \(t(G) = t(G')\) iff \(G' \in \mathcal{G}(G)\). Clearly, this is the most general classification task. Moreover, by replacing the target value \(t(G)\) with a probability \(p(G)\) (measure), the above task also encompasses generative tasks over \(\Omega\). All we need to show is that \(\bar{f}(G)\) of equation 1 is sufficiently expressive for the above task.

We now consider a permutation-sensitive function \(\bar{f}(A, X^{(v)})\) that assigns a distinct one-hot encoding to each distinct tensor \(A\) and node attribute sequence \(X^{(v)}\) inputs. This \(\bar{f}\) can be approximated arbitrarily well by a sufficiently expressive neural network (operating on the vector representation of the input) as these are known to be universal approximators (Hornik et al., 1989). Now, letting \(G' \in \Omega\) be arbitrary, for all \(G \in \mathcal{G}(G')\), we have

\[
\bar{f}(G) = \sum_{\pi \in \Pi_{|V|}} \bar{f}(A_{\pi,\pi}, X_{\pi}^{(v)}) = \sum_{(A', X^{(v)}) \in G} \bar{f}(A', X^{(v)}) = \bar{f}(G'),
\]

thus \(\bar{f}(G')\) is the unique fingerprint of the set \(G\). Then, all we need is a function \(\rho(\cdot)\) that takes the representation \(\bar{f}(G')\) and assigns the unique target value \(t(G')\), satisfying the desired condition and proving that RP has maximal representation power over \(\Omega\).
Proof of Theorem 2.2

Preliminaries. For an $n \times d_B$ matrix $B$ and an $n \times d_C$ matrix $C$, write $D = [B \times C]$ to denote their concatenation to form an $n \times (d_B + d_C)$ matrix $D$. Let $G_1 = (A_1, X_1^{(v)})$ and $G_2 = (A_2, X_2^{(v)})$ be two graphs with the same number of vertices $n$, otherwise the proof is trivial. Let $I_{|V|}$ be a $|V| \times |V|$ identity matrix representing the one-hot encoding vectors of node IDs 1 to $|V|$. Let $\alpha$ denote a maximally powerful WL-GNN, that is, a deep-enough WL-GNN satisfying the conditions of Theorem 3 in Xu et al. (2019). That is, the multiset functions for vertex aggregation and the graph-level readout are both injective over discrete node attributes.

Proof. We need to show that RP-GNN is strictly more expressive than WL-GNN. More specifically, we will show that RP-GNN (1) maps isomorphic graphs to the same embedding, (2) maps nonisomorphic graphs to distinct embeddings whenever a WL-GNN does, and (3) can successfully map some nonisomorphic graphs (that a WL-GNN cannot be represented as distinct by WP-GNN but cannot be represented as distinct by WL-GNN).

Let $G_1 = (A_1, X_1^{(v)})$ denote the graph $G_{\text{skip}}(M = 11, R = 2)$ and $G_2 = (A_2, X_2^{(v)})$ denote the graph $G_{\text{skip}}(M = 11, R = 3)$. It is easy to show that WL-GNN cannot give different representations to $G_1$ and $G_2$, as the WL test fails in these graphs (Arvind et al., 2017; Cai et al., 1992; Fürer, 2017) and the most powerful WL-GNN is just as powerful as the WL test (Xu et al., 2019).

To show RP-GNN is capable of giving different representations, we first show that for a given permutation $\pi$ of $G_1$, there is no permutation $\pi'$ of $G_2$ such that $\alpha((A_1)_\pi, (X_1^{(v)})_\pi \times I_{|V|}) = \alpha((A_2)_{\pi'}, (X_2^{(v)})_{\pi'} \times I_{|V|})$. In this part of the proof, for simplicity and without loss of generality, consider $\pi$ a permutation such that the vertices are numbered sequentially from $1, 2, \ldots, |V|$ clockwise around the circle in figure 1. Then, node $3$ in $G_1$ has neighbors $N_3 = \{1, 2, 4, 5\}$ and node $4$ has neighbors $N_4 = \{2, 3, 5, 6\}$, with intersection $N_3 \cap N_4 = \{2, 5\}$. In $G_2$, no two nodes share two neighbors, completing our proof of this claim.

Thus, there exists an $\alpha$ such that one layer of the GNN recursion in equation 4 maps $G_1$ and $\alpha((G_2)_\pi)$ to different embeddings, for all $\pi$ (this is easy to prove using lemma 5 of Xu et al. (2019) or even theorem 2 of Zaheer et al. (2017) as the node attributes are unique). As no representation of $G_2$ can match any representation of $G_1$, it is easy to find a function $g(\cdot)$ that, when composed with $\alpha$, ensures that the sum in equation 1 gives different values for $G_1$ and $G_2$. Because we can trivially re-define $\alpha' = g \circ \alpha$ and $\alpha'$ is still a WL-GNN, we conclude our proof.

Proof of Proposition 2.2

We restate the proposition for completeness.

Proposition. The RP in equation 10 requires summing over all $k$-node induced subgraphs of $G$, thus saving computation when $k < |V|$, reducing the number of terms in the sum from $|V|!$ to $\frac{|V|!}{(|V|-k)!}$. 

Proof. $k$-ary RP needs to iterate over the $k$-node induced subgraphs of $G$ ($\binom{|V|}{k}$ subgraphs), but for each subgraph there are $k!$ different ways to order its nodes, resulting in $\binom{|V|}{k} k!$ evaluations of $f$. 

Proof of Proposition 2.3

We restate the theorem for completeness.

**Proposition.** \( \overline{f}^{(k)} \) becomes strictly more expressive as \( k \) increases. That is, for any \( k \in \mathbb{N} \), define \( F_k \) as the set of all permutation-invariant graph functions that can be represented by RP with \( k \)-ary dependencies. Then, \( F_{k-1} \) is a proper subset of \( F_k \) if \( k \leq |V| \). Thus, RP with \( k \)-ary dependencies can express any RP function with \((k-1)\)-ary dependencies, but the converse does not hold.

**Proof.** \((F_{k-1} \subset F_k)\): Consider an arbitrary element \( \overline{f}^{(k-1)} \in F_{k-1} \), and write \( \overline{f} \left( A[1 : (k-1), 1 : (k-1), :], X^{(v)}[1 : (k-1), :] ; W \right) \) for its associated permutation-sensitive RP function. Consider \( \overline{f}^{(k)} \in F_k \) and let \( \overline{f}' \) be its associated permutation-sensitive RP function. For any tensor \( A \) (and attribute matrix \( X^{(v)} \)), we can define \( \overline{f}' \left( A[1:k, 1:k, :], X^{(v)}[1:k, :] ; W \right) = \overline{f} \left( A[1 : (k-1), 1 : (k-1), :] ; W \right) \). Thus, \( \overline{f}^{(k-1)} \in F_k \) and because \( \overline{f}^{(k-1)} \) is arbitrary, we conclude \( F_{k-1} \subset F_k \).

\((F_k \not\subset F_{k-1})\): The case where \( k = 1 \) is trivial, so assume \( k > 1 \). We will demonstrate \( \exists \overline{f}^{(k)} \in F_k \) such that \( \overline{f}^{(k)} \not\in F_{k-1} \). Let \( \overline{f}^{(k)} \) and \( \overline{f}^{(k-1)} \) be associated with \( \overline{f}^{(k)} \) and \( \overline{f}^{(k-1)} \), respectively.

**Task.** Consider the task of representing the class of circle graphs with skip links shown in figure 1 (with \( X^{(v)} = c1 \) for some \( c \in \mathbb{R} \)). Let \( G_k \in \mathcal{G}_{\text{skip}}(M_k, k) \) and \( G_{k+1} \in \mathcal{G}_{\text{skip}}(M_k, k + 1) \) where \( M_k \) is any prime number satisfying \( M_k > 2(k-1)(k+1) \). That is, \( G_k \) and \( G_{k+1} \) are countable skip length graphs with the same number of vertices and skip lengths of \( k \) and \( k + 1 \), respectively. Note that \( M_k > k + 1 \) is prime and thus it is coprime with both \( k \) and \( k + 1 \); further, \( M_k - 1 > k + 1 \) and the conditions for creating the CSL graph in definition 4.1 are satisfied. All \( w \) need is to show that there is a \( \overline{f}^{(k)} \) capable of distinguishing \( G_k \) from \( G_{k+1} \) but no such \( \overline{f}^{(k-1)} \) exists.

A \( k \)-ary \( \overline{f}^{(k)} \) that can distinguish between \( G_k \) and \( G_{k+1} \).

We will define \( \overline{f}^{(k)} \) in terms of a composition with a canonical orientation that numbers the vertices consecutively clockwise around the circle. Formally, in this orientation the elements of the adjacency matrix immediately next to the diagonal (\( A_{1, i+1} \) and \( A_{i, i-1} \)) are 1, which does not hold for other orientations. Thus, define \( \overline{f}^{(k)}(A_{\pi, \pi}[1 : k, 1 : k, :], X^{(v)}[1 : k, :] ; W) = 0 \) for all those permutations that do not satisfy this orientation.

Under this orientation, we can easily construct a \( \overline{f}^{(k)} \) that can distinguish \( G_k \) from \( G_{k+1} \): in \( G_k \) the \( k \times k \) submatrices of \( A_k \) will have more nonzero elements. By construction, the induced subgraph of size \( k \) in \( G_k \) (under this orientation) will include a pair of vertices that are \( k \) ‘hops’ away and thus there will be an extra edge between them. In \( G_{k+1} \), the skip length is too long and thus the induced subgraphs of size \( k \) will have fewer edges.

No \((k-1)\)-ary \( \overline{f}^{(k-1)} \) can distinguish between \( G_k \) and \( G_{k+1} \). The induced subgraphs of size \( k-1 \) are “the same” in both \( G_k \) and \( G_{k+1} \), which implies that no satisfactory \( \overline{f}^{(k-1)} \) can be constructed. In particular, if we denote by \( \mathcal{L}_{k-1}(G_k) \) the multiset of induced subgraphs of size \( k-1 \) in \( G_k \) and by \( \mathcal{L}_{k-1}(G_{k+1}) \) the multiset of induced subgraphs of size \( k-1 \) in \( G_{k+1} \), it can be shown that \( \mathcal{L}_{k-1}(G_k) \) and \( \mathcal{L}_{k-1}(G_{k+1}) \) are equivalent in the following sense. There exists a bijection \( \phi \) between these finite multisets such that for every \( H \in \mathcal{L}_{k-1}(G_k) \), \( \phi(H) \in \mathcal{L}_{k-1}(G_{k+1}) \) is isomorphic to \( H \). For example, the multisets (with arbitrarily labeled vertices) \( \{ 0 \rightarrow 0 \rightarrow 0 , 0 \rightarrow 0 \rightarrow 0 \} \) and \( \{ 0 \rightarrow 0 , 0 \rightarrow 0 , 0 \rightarrow 0 \} \) have an isomorphism-preserving bijection between them and will thus be considered equal.

In the interest in space and brevity, what follows is a sketch. We observe that we only need to show that the multisets of ‘maximally connected’ induced subgraphs of size \( k-1 \) that include the vertex \( 0 \in V = \{ 0, 1, \ldots, M_k - 1 \} \) are equivalent in the sense of having an isomorphism-preserving bijection \( \phi \) between them. By ‘maximally connected’, we mean an induced subgraph of size \( k-1 \) such that no more edges from \( G_R, R \in \{ k, k + 1 \} \) can be added without adding a \( k \)-th vertex to the induced subgraph. We only need to consider one vertex \( v = 0 \) due to the vertex transitivity of the CSL graphs. Once we show that this holds for ‘maximally connected’ induced subgraphs of size \( k-1 \), it follows that it is true for all connected induced subgraphs of size \( k-1 \) since they can be formed by deleting any edge that does not render the induced subgraph disconnected. Then, viewing disconnected graphs as the disjoint union of connected components, a similar argument to the one applied for connected induced subgraphs can be used to complete the argument for any possible induced subgraph of size \( k - 1 \).

We can construct all such maximally connected subgraphs including \( 0 \in V \) in both \( G_R \) for \( R \in \{ k, k + 1 \} \) by forming recursive sequences on the integers \( \{ 0, 1, \ldots, M_k - 1 \} \) with addition \( \bmod M_k \) (see definition 4.1); the key difference in these sequences is whether \( R = k \) or \( R = k + 1 \) can be added to the previous value in the sequence. Distinct sequences may result in equivalent induced subgraphs but we simply take one representative from each equivalence.
Table 3: Datasets used in our experiments.

| Data Set | Number of Compounds | Number of Tasks |
|----------|---------------------|-----------------|
| HIV      | 41,127              | 1               |
| MUV      | 93,087              | 17              |
| Tox 21   | 6,284               | 12              |

class. But these sequences can be constructed in a way that abstracts from either underlying graph $G_k$ or $G_{k+1}$. Due to our choice of $M_k$, the recursive sequences never 'wrap around' the graph and can be (informally) thought as a recursive sequence on a 'line segment' with 0 in the middle. In particular, there is a bijective relabeling of each graph so that every maximal induced subgraph of size $k$ on $G_R$ including 0 can be formed by a recursive sequence on the set of integers between $-(k+1)(k-1)$ and $(k+1)(k-1)$ (inclusive) with regular addition. Then it becomes clear that there is a bijection between any recursive $(k+1)$-sequence and any $k$-sequence on this bounded interval of integers (any sequence defined in terms of adding or subtracting $k+1$ can be replaced by one that adds or subtracts $k$). This provides the isomorphism-preserving bijection $\phi$ that we need.

C. Further Details of the Experiments

C.1. Relational Pooling and Graph Structure Representation

Our GIN architecture uses five layers of recursion, where every MLP$(l)$ has two hidden layers with 16 neurons in the hidden layers. The graph embedding is mapped to the output through a final linear layer $\text{softmax}(h^2_\phi W)$, $e^{(l)}$ is treated as a learnable parameter. With standard GIN, since the vertex attributes are not one-hot encoded (they are constants), we first apply an MLP embedding before computing the first update recursion (as in Xu et al. (2019)). Since RP-GIN utilizes one-hot IDs, we do not need an MLP embedding in the first update. Figure 3 shows the stronger performance of RP-GIN on this task.

C.2. Predicting Molecular Properties

Here we provide additional details on the molecular experiments. (1) For the models based on Graph Convolution (Duvenaud et al., 2015), we extend the architecture provided from DeepChem and the MoleculeNet project. Following them, the learning rate was set to 0.003, we trained with mini-batches of size 96, and the Adam optimizer was used. Models were trained for 100 epochs. Training was performed on 48 CPUs using the inherent multithreading of DeepChem. (2) For the so-called RNN and CNN models, all MLPs have one hidden layer with 100 neurons. We used the Adam optimizer (Kingma & Ba, 2015), again training all models with mini-batches of size 96 and 100 epochs. We performed a hyperparameter line search over the learning rate, with values in $\{0.003, 0.001, 0.01, 0.03, 0.1, 0.3\}$. Training was performed on GeForce GTX 1080 Ti GPUs. To model the RNN, we use an LSTM with 100 neurons and use the long term memory as output.

When we train RP-Duvenaud, we follow any training particular as in the DeepChem implementation. For instance, DeepChem’s implementation computes a weighted loss which penalizes misclassification differently depending on the task, and they compute an overall performance metric by taking the mean of the ROC-AUC across all tasks (see Table 3). One difference is that the DeepChem recommends either metrics PRC-AUC or ROC-AUC and splits “random” or “scaffold” depending on the dataset under consideration. Since ROC-AUC and random splits were the most commonly used among the three datasets we chose, we decided – before training any models – to use random splits and ROC-AUC for every dataset for simplicity. We also note that the authors of MoleculeNet report ROC-AUC scores on all three datasets. Regarding the sizes of the train/validation/test splits, we used the default values provided by DeepChem.

To train with $\pi$-SGD, we sample a different random permutation of the graph at each forward pass. In the case of RP-Duvenaud, this involves assigning permutation-dependent unique IDs at each forward step (as in equation 5). In our implementation, we achieve this by building a new DeepChem object for the molecule at each forward pass. This operation is expensive but we did not consider refined code optimizations for this work. Therefore, training the models on MUV was expensive and we were only able to run for 10 random data splits as opposed to 20 for the others. In general, with properly optimized code, sampling permutations need not be as expensive and allows for a tractable and theoretically justified procedure.

We implement the model that assigns unique IDs to atoms by first finding the molecule with the most atoms across training, validation, and test sets, and then appending a feature vector of that size to the endowed vertex attributes. That is, if the largest molecule has $A$ atoms, we concatenate a vector of length $A$ of one-hot IDs to the existing vertex attributes (for every vertex in each molecule). Looking ahead to the test data in order to find the largest molecule in test and validation corresponds to using domain knowledge and the modeling choice that the resulting model will only work on molecules with at most $A$ atoms. It is not hard to construct a similar model that does not rely on this look-ahead mechanism, such as assigning a one-hot encoding of $i \mod A_{observed}$ where $i \in \{1, 2, \ldots, |V|\}$ and $A_{observed}$ is the largest molecule observed in the model building phase.
Figure 4: Training time and model performance of $k$-ary models for the Tox21 task. Test-set AUC was computed for five different random splits of train/validation/test: we show the mean ± one standard deviation. We also show the speed up factor for training: time to train on the full graph by time for $k$-ary model. Training was performed on 48 CPUs, making use of PyTorch’s inherent multithreading.

Figure 5: Training time and model performance of $k$-ary models for the MUV task.

Figure 6: Training time and model performance of $k$-ary models for the HIV task.