Understanding and Extending Subgraph GNNs by Rethinking Their Symmetries

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Abstract

Subgraph GNNs are a recent class of expressive Graph Neural Networks (GNNs) which model graphs as collections of subgraphs. So far, the design space of possible Subgraph GNN architectures as well as their basic theoretical properties are still largely unexplored. In this paper, we study the most prominent form of subgraph methods, which employs node-based subgraph selection policies such as ego-networks or node marking and deletion. We address two central questions: (1) *What is the upper-bound of the expressive power of these methods?* and (2) *What is the family of equivariant message passing layers on these sets of subgraphs?*. Our first step in answering these questions is a novel symmetry analysis which shows that modelling the symmetries of node-based subgraph collections requires a significantly smaller symmetry group than the one adopted in previous works. This analysis is then used to establish a link between Subgraph GNNs and Invariant Graph Networks (IGNs). We answer the questions above by first bounding the expressive power of subgraph methods by 3-WL, and then proposing a general family of message-passing layers for subgraph methods that generalises all previous node-based Subgraph GNNs. Finally, we design a novel Subgraph GNN dubbed `SUN`, which theoretically unifies previous architectures while providing better empirical performance on multiple benchmarks.

1 Introduction

Message Passing Neural Networks (MPNNs) are arguably the most commonly used version of Graph Neural Networks (GNNs). The limited expressive power of MPNNs [31, 45] has led to a plethora of works aimed at designing expressive GNNs while maintaining the simplicity and scalability of MPNNs [9, 34, 40, 25]. Several recent studies have proposed a new class of such architectures [12, 49, 6, 50, 37, 36], dubbed *Subgraph GNNs*, which apply MPNNs to collections ('bags') of subgraphs extracted from the original input graph and then aggregate the resulting representations. Subgraphs are selected according to a predefined policy; in the most popular ones, each subgraph is tied to a specific node in the original graph, for example by deleting it or extracting its local ego-network. Subgraph GNNs have demonstrated outstanding empirical performance, with state-of-the-art results on popular benchmarks like the ZINC molecular property prediction [50, 6].

While offering great promise, it is fair to say that we still lack a full understanding of Subgraph GNNs. Firstly, on the theoretical side, it is known that subgraph methods are

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strictly stronger than the Weisfeiler-Leman (WL) test [44, 34], but an upper-bound on their expressive power is generally unknown. Secondly, on a more practical level, Subgraph GNN architectures differ considerably in the way information is aggregated and shared across the subgraphs, and an understanding of the possible aggregation and sharing rules is missing. Both aspects are important: an understanding of the former can highlight the limitations of emerging architectures, a study of the latter paves the way for improved Subgraph GNNs.

Main contributions. The goal of this paper is to provide a deeper understanding of node-based Subgraph GNNs in light of the two aforementioned aspects. The main theoretical tool underpinning our contributions is a novel analysis of the symmetry group that acts on the sets of subgraphs. While several previous approaches [37, 12, 6] have (often implicitly) assumed that a subgraph architecture should be equivariant to independent node and subgraph permutations, we leverage the fact that node-based policies induce an inherent bijection between the subgraphs and the nodes. This observation allows us to align the two groups and model the symmetry with a single (smaller) permutation group that acts on nodes and subgraphs *jointly*. Other works [50, 46, 49] have (again, implicitly) recognised such node-subgraph correspondence but without studying the implications on the symmetry group, and resorting, as a result, to a partial and heuristic choice of equivariant operations.

The use of this stricter symmetry group raises a fruitful connection with k-order Invariant Graph Networks (`k-IGN`s) [28, 27], a well studied family of architectures for processing graphs and hypergraphs designed to be equivariant to the same symmetry group. This connection allows us to transfer and reinterpret previous results on `IGN`s to our Subgraph GNN setup. As our first contribution we show that the expressive power of Subgraph GNNs with node-based policies is bounded by that of the `3-WL` test. This is shown by proving that all previous Subgraph GNNs can be implemented by a `3-IGN` and by leveraging the fact that the expressive power of these models is known to be bounded by `3-WL` [18, 4].

Our second contribution is the proposal of a general layer formulation for Subgraph GNNs, based on the observation that these methods maintain an $n \times n$ representation of n subgraphs with n nodes, following the same symmetry structure of `2-IGN`s (same permutation applied to both rows and columns of this representation). We propose a novel extension of `2-IGN`s capturing both local (message-passing-like) and global operations. This extension easily recovers previous methods and facilitates their comparison. In addition, we present a number of new operations that previous methods did not implement. We build upon these observations in order to devise a new Subgraph GNN dubbed `SUN`, (*Subgraph Union Network*). We prove that `SUN` generalises all previous node-based Subgraph GNNs and we comprehensively compare its empirical performance to these methods, showing it can outperform them.

2 Previous work

Expressive power of GNNs. The expressive power of GNNs is a central research focus since it was realised that message-passing type GNNs are constrained by the expressivity of the WL isomorphism test [31, 45]. Numerous approaches for more powerful GNNs have been proposed, including positional and structural encodings [1, 38, 9, 15, 24, 26], higher-order message passing schemes [31, 33, 8, 7], and equivariant models [21, 28, 27, 43, 13, 42, 35]. We refer readers to the recent survey by Morris et al. [34] for additional details.

Invariant graph networks. `IGN`s were recently introduced in a series of works by Maron et al. [28, 27, 29] as an alternative to MPNNs for processing graph and hyper-graph data. For $k \geq 2$, `k-IGN`s use k-order tensor representations $\mathbb{R}^{n^k}$ and apply linear S_n-equivariant layers interspersed with pointwise nonlinearities. `IGN`s were shown to have the same expressive power as the `k-WL` graph isomorphism test [27, 4, 18]. For sufficiently large k, these models have a universal approximation property w.r.t. S_n-invariant and equivariant functions [29, 22, 39]. As Maron et al. [28] showed that the dimension of a basis for linear equivariant layers between

k-order representations is super-exponential (bell$(2k)$), for $k > 3$ these models currently remain of mostly theoretical value, due to their computational complexity. Albooyeh et al. [2] showed that such linear equivariant layers can be written as sums of pooling and broadcasting operations between orbits of S_n on $\{1, \ldots, n\}^k$. Morris et al. [34] provide a review of `IGN`s.

3 Subgraph GNNs

Notation. Let $G = (A, X)$ be a member of the family $\mathcal{G}$ of *node-attributed*, undirected, finite, simple graphs[1]. The *adjacency matrix* $A \in \mathbb{R}^{n \times n}$ represents G's edge set E over its set of n nodes V. The *feature matrix* $X \in \mathbb{R}^{n \times d}$ gathers the node features; we denote by $x_j \in \mathbb{R}^{d \times 1}$ the features of node j corresponding to the j-th row of X. B_G is used to denote a multiset (bag) of m subgraphs of G. Adjacency and feature matrices for subgraphs in B_G are arranged in tensors $\mathcal{A} \in \mathbb{R}^{m \times n \times n}$ and $\mathcal{X} \in \mathbb{R}^{m \times n \times d}$. Superscript $^{i,(t)}$ refers to representations on subgraph i at the t-th layer of a stacking, as in $x_j^{i,(t)}$. Finally, we denote $[n] = \{1, \ldots, n\}$. All proofs are deferred to Appendix B and D.

Formalising Subgraph GNNs. Subgraph GNNs compute a representation of $G \in \mathcal{G}$ as

$$(A, X) \mapsto \big(\mu \circ \rho \circ \mathcal{S} \circ \pi\big)(A, X). \tag{1}$$

Here, $\pi : G \mapsto \{G^1, ..., G^m\} = \{(A^1, X^1), ..., (A^m, X^m)\} = B_G^{(0)}$ is a *selection policy* generating a bag of subgraphs from G; $\mathcal{S} = L_T \circ \ldots \circ L_1 : B_G^{(0)} \mapsto B_G^{(T)}$ is a *stacking* of T (node- and subgraph-) permutation equivariant layers; $\rho : (G, B_G^{(T)}) \mapsto x_G$ is a permutation invariant *pooling function*, μ is an MLP. Subgraph GNNs differ in the implementation of π, $\mathcal{S}$ and, in some cases, ρ. For example, in 1-Reconstruction GNNs [12], π selects node-deleted subgraphs and $\mathcal{S}$ applies a Siamese MPNN to each subgraph independently. To exemplify the variability in $\mathcal{S}$, ESAN [6] extends this method with cross-subgraph node and connectivity aggregation. Layers in $\mathcal{S}$ comprise a *base-encoder* in the form of a GNN applied to subgraphs; throughout this paper, we assume it to be a `1-WL` maximally expressive MPNN such as the one in [31].

Node-based selection policies. In this work, we focus on a specific family of *node-based* subgraph selection policies, wherein every subgraph is associated with a unique node in the graph. Formally, we call a subgraph selection policy *node-based* if it is of the form $\pi(G) = \{f(G, v)\}_{v \in V}$, for some *selection function* $f(G, v)$ that takes a graph G and a node v as inputs and outputs a subgraph G^v. In the following, we refer to v as the *root* of subgraph G^v. We require f to be a bijection and we note that such policies produce $m = n$ different subgraphs. Amongst the most common examples are *node-deletion* (ND), *node-marking* (NM), and *ego-networks* (EGO) policies. For input graph G, $f_{\text{ND}}(G, v)$ removes node v and the associated connectivity; $f_{\text{NM}}(G, v)$ adds a special 'mark' attribute to v's features (with no connectivity alterations), and $f_{\text{EGO}(h)}(G, v)$ returns the subgraph induced by the h-hop-neighbourhood around the root v. EGO policies can be 'marked': $f_{\text{EGO+}(h)}(G, v)$ extracts the h-hop ego-net around v *and* marks this node as done by f_{NM}. For convenience, we denote the class of such node-based selection policies by Π:

Definition 1 (Known node-based selection policies Π)**.** *Let Σ be the set of all node-based subgraph selection policies. Class $\Pi \subset \Sigma$ collects the node-based policies node-deletion (ND), node-marking (NM), ego-nets (EGO) and marked ego-nets (EGO+) of any depth:* $\Pi = \{\pi_{\text{ND}}, \pi_{\text{NM}}, \pi_{\text{EGO}(h)}, \pi_{\text{EGO+}(h)} \mid h > 0\}$.

Appendix A presents the different formulations of currently known node-based Subgraph GNNs in detail, which we group in the the following family of models:

Definition 2 (Known Subgraph GNNs Υ)**.** *Let Ξ be the set of all node-based Subgraph GNNs. Class $\Upsilon \subset \Xi$ collects known Subgraph GNNs when equipped with `1-WL` base-encoders:* $\Upsilon = \{$1-Reconstr.GNN, DS-GNN, DSS-GNN, GNN-AK, GNN-AK-ctx, NGNN, ID-GNN$\}$.

[1] We do not consider edge features, although an extension to such a setting would be possible.

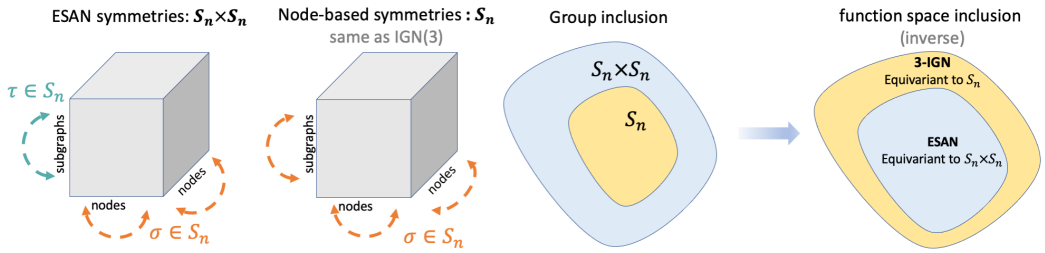


Figure 1: Symmetries of bags of subgraphs (left) and corresponding function space diagrams (right). In ESAN [6] symmetries are modelled as a direct product of node and subgraph permutation groups; however, node-based policies enable the use of one single permutation group, the same as in `3-IGN`s. `3-IGN`s are less constrained, thus more expressive than ESAN and other Subgraph GNNs. See diagram on the right and formal statement in Section 5.

Importantly, all these methods apply MPNNs to subgraphs of the original graph, but differ in the way information is shared between subgraphs/nodes. In all cases, their expressive power is strictly larger than `1-WL`, but an *upper*-bound is currently unknown.

4 Symmetries of node-based subgraph selection policies

In an effort to characterise the representational power of node-based Subgraph GNNs, we first study the symmetry group of the objects they process: 'bags of subgraphs' represented as tensors $(\mathcal{A}, \mathcal{X}) \in \mathbb{R}^{m \times n \times n} \times \mathbb{R}^{m \times n \times d}$, assuming n nodes across m subgraphs. Previous approaches [12, 6, 37] used two permutation groups: one copy of the symmetric group S_n models *node permutations*, while another copy S_m models *subgraph permutations* in the bag. These two were combined by a group product[2] acting *independently* on the nodes and subgraphs in $(\mathcal{A}, \mathcal{X})$. For example, Bevilacqua et al. [6] model the symmetry as:

$$((\tau, \sigma) \cdot \mathcal{A})_{ijk} = \mathcal{A}_{\tau^{-1}(i)\sigma^{-1}(j)\sigma^{-1}(k)}, \quad ((\tau, \sigma) \cdot \mathcal{X})_{ijl} = \mathcal{X}_{\tau^{-1}(i)\sigma^{-1}(j)l}, \qquad (\tau, \sigma) \in S_m \times S_n \quad (2)$$

Our contributions stem from the following crucial observation: When using node-based policies, the subgraphs in $(\mathcal{A}, \mathcal{X})$ can be *ordered consistently with the nodes* by leveraging the bijection $f : v \mapsto G_v$ characterising this policy class. In other words, f suggests a node-subgraph alignment inducing a new structure on $(\mathcal{A}, \mathcal{X})$, whereby the subgraph order is not independent of that of nodes anymore. Importantly, this new structure is preserved *only* by those permutations operating identically on both nodes and subgraphs. Following this observation, the symmetry of a node-based bag of subgraphs is modelled more accurately using only *one single permutation group* S_n jointly acting on both nodes and subgraphs:

$$(\sigma \cdot \mathcal{A})_{ijk} = \mathcal{A}_{\sigma^{-1}(i)\sigma^{-1}(j)\sigma^{-1}(k)}, \quad (\sigma \cdot \mathcal{X})_{ijl} = \mathcal{X}_{\sigma^{-1}(i)\sigma^{-1}(j)l}, \qquad \sigma \in S_n \quad (3)$$

It should be noted that S_n is *significantly smaller* than $S_n \times S_n$[3]. Informally, the latter group contains many permutations which are not in the former: those acting differently on nodes and subgraphs and, thus, not preserving the new structure of $(\mathcal{A}, \mathcal{X})$. Since they are restricted by a smaller set of equivariance constraints, we expect GNNs designed to be equivariant to S_n to be be more expressive than those equivariant to the larger groups considered by previous works [29]. See Figure 1 for an illustration.

The insight we obtain from Equation (3) is profound: it reveals that the symmetry structure of $\mathcal{A}$ exactly matches the symmetries of third-order tensors used by `3-IGN`s, and similarly, that the symmetry structure for $\mathcal{X}$ matches the symmetries of second-order tensors used by `2-IGN`s. In the following, we will make use of this insight and the fact that `IGN`s are well-studied objects to prove an upper-bound on the expressive power of Subgraph GNNs and to design principled extensions to these models.

[2] Bevilacqua et al. [6] use a direct-product, assuming nodes in subgraphs are consistently ordered. Cotta et al. [12] use the larger wreath-product assuming node ordering in the subgraph is unknown.

[3] More formally, S_n's orbits on the indices in (3) refine the orbits of the product group in (2).

5 A representational bound for Subgraph GNNs

In this section we prove that the expressive power of known node-based Subgraph GNNs is bounded by `3-WL` by showing that they can be implemented by `3-IGN`s, which have the same expressive power as `3-WL`. Underpinning the possibility of `IGN`s to upper-bound a certain Subgraph GNN $\mathcal{N}$ in its expressive power is the ability of `IGN`s to (i) implement $\mathcal{N}$'s subgraph selection policy (π) and (ii) implement $\mathcal{N}$'s (generalised) message-passing and pooling equations ($\mu \circ \rho \circ \mathcal{S}$). This would ensure that whenever $\mathcal{N}$ assigns distinct representations to two non-isomorphic graphs, an `IGN` implementing $\mathcal{N}$ would do the same. We start by introducing a basic, useful concept that will often recur in the following sections.

Definition 3 ("implements"). *Let $f : D_f \to C_f$, $g : D_g \to C_g$ be two functions and such that $D_g \subseteq D_f, C_g \subseteq C_f$. We say f* implements *g (and write $f \cong g$) when $\forall x \in D_g, f(x) = g(x)$.*

Our first result shows that `3-IGN`s can implement the selection policies in class Π (Definition 1), which, to the best of our knowledge, represent *all known* node-based policies utilised by previously proposed Subgraph GNNs.

Lemma 4 (`3-IGN`s implement known selection policies). *For any $\pi \in \Pi$ there exists a stacking of `3-IGN` layers $\mathcal{M}_\pi$ s.t. $\mathcal{M}_\pi \cong \pi$.*

Intuitively, `3-IGN`s start from a $\mathbb{R}^{n^2}$ representation of G and, first, move to a $\mathbb{R}^{n^3}$ tensor 'copying' this latter along its first (subgraph) dimension. This is realised via an appropriate broadcast operation. Then, they proceed by adding a 'mark' to the features of some nodes and/or by nullifying elements corresponding to some edges. Next, we show that `3-IGN`s can implement the layers of any subgraph model $\mathcal{N} \in \Upsilon$.

Lemma 5 (`3-IGN`s implement Subgraph GNN layers). *Let G_1, G_2 be two graphs in $\mathcal{G}$ and $\mathcal{N}$ a model in family Υ equipped with Morris et al. [31] message-passing base-encoders. Let $B_1^{(t)}, B_2^{(t)}$ be bags of subgraphs in the input of some intermediate layer L in $\mathcal{N}$. Then there exists a stacking of `3-IGN` layers $\mathcal{M}_L$ for which $\mathcal{M}_L(B_i^{(t)}) = B_i^{(t+1)} = L(B_i^{(t)})$ for $i = 1, 2$.*

Lemmas 4 and 5 allow us to upper-bound the expressive power of all known instances of node-based Subgraph GNNs by that of `3-IGN`s:

Theorem 6 (`3-IGN`s upper-bound Subgraph GNNs). *For any pair of non-isomorphic graphs G_1, G_2 in family $\mathcal{G}$ and Subgraph GNN model $\mathcal{N} \in \Upsilon$ equipped with Morris et al. [31] message-passing base-encoders, if there exists weights Θ such that G_1, G_2 are distinguished by instance $\mathcal{N}_\Theta$, then there exist weights Ω for a 3-IGN instance $\mathcal{M}_\Omega$ such that G_1, G_2 are distinguished by $\mathcal{M}_\Omega$ as well.*

Theorem 6 has profound consequences in the characterisation of the expressive power of node-based Subgraph GNNs, as we show in the following

Corollary 7 (`3-WL` upper-bounds Subgraph GNNs). *Let $G_1, G_2 \in \mathcal{G}$ be two non-isomorphic graphs and $\mathcal{N}_\Theta \in \Upsilon$ one instance of model $\mathcal{N}$ with weights Θ. If $\mathcal{N}_\Theta$ distinguishes G_1, G_2, then the `3-WL` algorithm does so as well.*

Proof idea: If there is a pair of graphs undistinguishable by `3-WL`, but for which there exists a Subgraph GNN separating them, there must exists a `3-IGN` separating these (Theorem 6). This is in contradiction with the result in Geerts [18], Azizian and Lelarge [4].

6 A design space for Subgraph GNNs

As discussed, different formulations of Subgraph GNNs differ primarily in the specific rules for updating node representations across subgraphs. However, until now it is not clear whether existing rules exhaust all the possible equivariant options. We devote this section to a systematic characterisation of the 'layer space' of Subgraph GNNs.

In the spirit of the previous Section 5, where we "embedded" Subgraph GNNs in `3-IGN`s, one option would be to consider all $\text{bell}(6) = 203$ linear equivariant operations prescribed by this formalism. However, this choice would be problematic for three main reasons: (i) This layer space is *too vast* to be conveniently explored; (ii) It includes operations involving $\mathcal{O}(n^3)$ space complexity, impractical in most applications; (iii) The linear `IGN` basis does not directly support local message passing, a key operation in Subgraph methods. Following previous Subgraph GNN variants, which use $\mathcal{O}(n^2)$ storage for the representation of n nodes in n subgraphs, we set the desideratum of $\mathcal{O}(n^2)$ memory complexity as our main constraint, and use this restriction to reduce the design space. To be more precise, we are interested in modelling S_n-equivariant transformations on the subgraph-node tensor $\mathcal{X}$.

6.1 Extended 2-IGNs

As we have already observed in Equation 3 in Section 4, such a second order tensor $\mathcal{X}$ abides by the same symmetry structure of `2-IGN`s. We therefore gain intuition from the characterisation of linear equivariant mappings as introduced by Maron et al. [28], and propose an extension of this formalism.

`2-IGN` layer space. A `2-IGN` layer L_Θ updates $\mathcal{X} \in \mathbb{R}^{n\times n\times d}$ as $\mathcal{X}^{(t+1)} = L_\Theta\big(\mathcal{X}^{(t)}\big)$ by applying a specific transformation to on- (x_i^i) and off-diagonal terms $(x_j^i, i \neq j)$:

$$x_i^{i,(t+1)} = \upsilon_{\theta_1}\big(x_i^{i,(t)}, \underset{j}{\square}\, x_j^{j,(t)}, \underset{j\neq i}{\square}\, x_j^{i,(t)}, \underset{h\neq i}{\square}\, x_i^{h,(t)}, \underset{h\neq j}{\square}\, x_j^{h,(t)}\big) \tag{4}$$

$$x_i^{k,(t+1)} = \upsilon_{\theta_2}\big(x_i^{k,(t)}, x_k^{i,(t)}, \underset{h\neq j}{\square}\, x_j^{h,(t)}, \underset{h\neq i}{\square}\, x_i^{h,(t)}, \underset{j\neq k}{\square}\, x_j^{k,(t)}, \underset{j\neq i}{\square}\, x_j^{i,(t)}, \underset{h\neq k}{\square}\, x_k^{h,(t)}, x_k^{k,(t)}, x_i^{i,(t)}, \underset{j}{\square}\, x_j^{j,(t)}\big)$$

Here, $\square$ indicates a permutation invariant aggregation function, $\upsilon_{\theta_1}, \upsilon_{\theta_2}$ apply a specific $d \times d'$ linear transformation to each input term and sum the outputs including bias terms.

`ReIGN(2)` layer space. As `2-IGN` layers are linear, the authors advocate setting $\square \equiv \sum$, performing pooling as *global* summation. Here, we extend this formulation to additionally include different *local* aggregation schemes. In this new extended formalism, entry x_i^k represents node i in subgraph k; accordingly, each aggregation in Equation 4 can be also performed locally, i.e. extending only over i's neighbours, as prescribed by the connectivity of subgraph k or of the original input graph. As an example, when updating entry $x_i^{k,(t)}$, term $\square_{j\neq k}\, x_j^{k,(t)}$ is expanded as $\big(\square_{j\neq k}\, x_j^{k,(t)}, \square_{j\sim_k i}\, x_j^{k,(t)}, \square_{j\sim i}\, x_j^{k,(t)}\big)$, with $\sim_k$ denoting adjacency in subgraph k, and $\sim$ that in the original graph connectivity. Each term in the expansion is associated with a specific learnable linear transformation. We report a full list of pooling operations in Appendix D, Table 3. These local pooling operations allow to readily recover sparse message passing, which constitutes the main computational primitive of all popular (Subgraph) GNNs. We also note that other characteristic Subgraph GNN operations are also recovered by this formalism: for example, $\square_{h\neq i}\, x_i^{h,(t)}$ operates global pooling of node i's representations across subgraphs, as previously introduced in Bevilacqua et al. [6], Zhao et al. [50]. We generally refer to this framework as `ReIGN(2)` ("Rethought `2-IGN`").

`ReIGN(2)` architectures. `ReIGN(2)` induces (linear) layers in the same form of Equation 4, but where $\square$ terms are expanded to both local and global operations, as explained. These layers can operate on any bag generated by a node-based selection policy $\bar{\pi}$, and can be combined together in `ReIGN(2)` stacks of the form $\mathcal{S}_\mathcal{R} = L^{(T)} \circ \sigma \circ L^{(T-1)} \circ \sigma \circ \ldots \circ \sigma \circ L^{(1)}$, where σ's are pointwise nonlinearities and L's are `ReIGN(2)` layers. This allows us to define `ReIGN(2)` models as Subgraph GNNs in the form of Equation 1, where $\mathcal{S}$ is a `ReIGN(2)` layer stacking and π is node-based: $\mathcal{R}_{\bar{\pi}} = \mu \circ \rho \circ \mathcal{S}_\mathcal{R} \circ \bar{\pi}$.

More generally, `ReIGN(2)` induces a 'layer space' for node-based Subgraph GNNs: the expanded terms in its update equations represent a pool of atomic operations that can be selected and combined to define new equivariant layers. Compared to that of `3-IGN`s, this space is of tractable size, yet recovers previously proposed Subgraph GNNs and allows to define novel interesting variants, as we will show next.

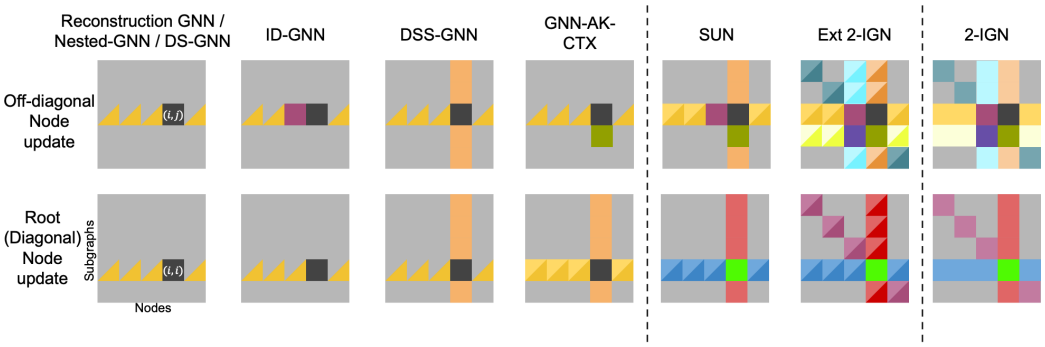


Figure 2: A comparison of aggregation and update rules in Subgraph GNNs, illustrated on an $n \times n$ matrix holding n subgraphs with n node features. Top row shows off-diagonal updates, bottom row shows diagonal (root node) updates. Each color represents a different parameter. Full squares represent global sum pooling; triangles represent local pooling. Two triangles represent both local and global pooling. See Appendix C for more details.

Recovering previous Subgraph GNNs. The following result states that the introduced formalism generalises all known node-based Subgraph GNN architectures, as their layers are captured by a `ReIGN(2)` stacking.

Theorem 8. *Let $\mathcal{N}$ be a model in family Υ equipped with Morris et al. [31] message-passing base-encoders. For any instance $\mathcal{N}_\Theta$, there exists `ReIGN(2)` instance $\mathcal{R}_\Omega$ such that $\mathcal{R}_\Omega \cong \mathcal{N}_\Theta$.*

This shows that known methods are generalised without resorting to the $\mathcal{O}(n^3)$ computational complexity of `3-IGN`s. Figure 2 illustrates the aggregation and sharing rules used by previous subgraph GNNs, visually demonstrating how `ReIGN(2)` generalises previous methods. It is important to notice that, when employing policies in Π and `3-IGN`-computable invariant pooling functions ρ (as those used by models in Υ), `ReIGN(2)`s are upper-bounded by `3-IGN`s:

Proposition 9. *For any pair of non-isomorphic graphs G_1, G_2 in family $\mathcal{G}$, if there exist policy $\bar{\pi} \in \Pi$, parameters Θ and `3-IGN`-computable invariant pooling function ρ such that the `ReIGN(2)` instance $\mathcal{R}_{\rho,\Theta,\bar{\pi}}$ distinguishes G_1, G_2, then there exist weights Ω for a `3-IGN` instance $\mathcal{M}_\Omega$ such that G_1, G_2 are distinguished by $\mathcal{M}_\Omega$ as well.*

This proposition entails an upper-bound on the expressive power of `ReIGN(2)`.

Corollary 10. *The expressive power of a `ReIGN(2)` model with policy $\pi \in \Pi$ and `3-IGN`-computable invariant pooling function ρ is upper-bounded by `3-WL`.*

We note that there may be layers equivariant to S_n over $\mathbb{R}^{n^2}$ not captured by `ReIGN(2)`. Yet, previously proposed Subgraph GNN layers do not exhaust the `ReIGN(2)` design space, which remains largely unexplored. One, amongst possible novel constructions, is introduced next.

6.2 A unifying architecture: Subgraph Union Networks

We now show how the `ReIGN(2)` layer space can guide the design of novel, expressive, Subgraph GNNs. Our present endeavour is to conceive a computationally tractable architecture subsuming known node-based models: in virtue of this latter desideratum, we will dub this architecture "Subgraph Union Network" (`SUN`). To design the base equivariant layer for `SUN`, we select and combine specific aggregation terms suggested by the `ReIGN(2)` framework:

$$x_i^{i,(t+1)} = \sigma\Big(\upsilon_{\theta_1}\big(x_i^{i,(t)}, \sum_{j\sim_i i} x_j^{i,(t)}, \sum_j x_j^{i,(t)}, \sum_h x_i^{h,(t)}, \sum_{j\sim i}\sum_h x_j^{h,(t)}\big)\Big) \tag{5}$$

$$x_i^{k,(t+1)} = \sigma\Big(\upsilon_{\theta_2}\big(x_i^{k,(t)}, \sum_{j\sim_k i} x_j^{k,(t)}, x_i^{i,(t)}, x_k^{k,(t)}, \sum_j x_j^{k,(t)}, \sum_h x_i^{h,(t)}, \sum_{j\sim i}\sum_h x_j^{h,(t)}\big)\Big) \tag{6}$$

where υ's sum their inputs after applying a specific linear transformations to each term. One of the novel features of `SUN` is that roots are transformed by a *different set of parameters*

Table 1: Test mean MAE on the Counting Substructures and ZINC-12k datasets. All Subgraph GNNs employ a GIN base-encoder.

Method	Counting Substructures (MAE ↓)			
	Triangle	Tailed Tri.	Star	4-Cycle
GCN [23]	0.4186	0.3248	0.1798	0.2822
GIN [45]	0.3569	0.2373	0.0224	0.2185
PNA [11]	0.3532	0.2648	0.1278	0.2430
PPGN [27]	0.0089	0.0096	0.0148	**0.0090**
GNN-AK [50]	0.0934	0.0751	0.0168	0.0726
GNN-AK-CTX [50]	0.0885	0.0696	0.0162	0.0668
GNN-AK+ [50]	0.0123	0.0112	0.0150	0.0126
SUN (EGO)	0.0092	0.0105	0.0064	0.0140
SUN (EGO+)	**0.0079**	**0.0080**	**0.0064**	0.0105

Method	ZINC (MAE ↓)
GCN [23]	0.321± 0.009
GIN [45]	0.163 ± 0.004
PNA [11]	0.133 ± 0.011
GSN [9]	0.101 ± 0.010
CIN [7]	**0.079** ± 0.006
NGNN [49]	0.111 ± 0.003
DS-GNN (EGO) [6]	0.115 ± 0.004
DS-GNN (EGO+) [6]	0.105 ± 0.003
DSS-GNN (EGO) [6]	0.099 ± 0.003
DSS-GNN (EGO+) [6]	0.097 ± 0.006
GNN-AK [50]	0.105 ± 0.010
GNN-AK-CTX [50]	0.093 ± 0.002
GNN-AK+ [50]	0.086 ± ???
SUN (EGO)	0.083 ± 0.003
SUN (EGO+)	0.084 ± 0.002

(θ_1) than the other nodes [4] (θ_2, see Figure 2). In practice, the first and last two terms in each one of Equations (5) and (6) can be processed by maximally expressive MPNNs [31, 45], the remaining terms by MLPs. We test these variants in our experiments, with their formulations in Appendix G. `SUN` remains an instantiation of the `ReIGN(2)` framework:

Proposition 11 (A `ReIGN(2)` stacking implements `SUN` layers)**.** *For any `SUN` layer L defined according to Equations 5 and 6, there exists a `ReIGN(2)` layer stacking $\mathcal{S}_L$, such that $\mathcal{S}_L \cong L$.*

Finally, we show that a stacking of `SUN` layers can implement any layer of known node-based Subgraph Networks, making this model a principled generalisation thereof.

Proposition 12 (A `SUN` stacking implements known Subgraph GNN layers)**.** *Let $\mathcal{N}$ be a model in family Υ employing Morris et al. [31] as a message-passing base-encoder. Then, for any layer L in $\mathcal{N}$, there exists a stacking of `SUN` layers $\mathcal{S}_L$ such that $\mathcal{S}_L \cong L$.*

Beyond `SUN`. As it can be seen in Figure 2, `SUN` does not use all possible operations in the `ReIGN(2)` framework. Notably, two interesting operations that are not a part of `SUN` are: (i) The 'transpose': $x_i^k = \upsilon_\theta(x_k^i)$, which shares information between the i-th node in the k-th subgraph and the k-th node in the i-th subgraph; (ii) Local vertical pooling $x_i^k = \upsilon_\theta(\sum_{h \sim i} x_i^h)$. The exploration of these and other operations is left to future work.

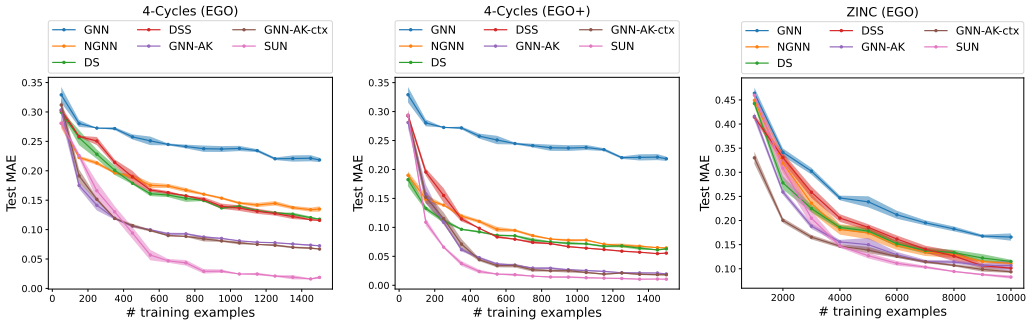
7 Experiments

We experimentally validate the effectiveness of one `ReIGN(2)` instantiation, comparing `SUN` to previously proposed Subgraph GNNs. We seek to verify whether its theoretical representational power practically enables superior accuracy in expressiveness tasks and real-world benchmarks. Concurrently, we pay attention to the *generalisation ability* of models in comparison. `SUN` layers are less constrained in their weight sharing pattern, resulting in a more complex model. As this is traditionally associated with inferior generalisation abilities in low data regimes, we deem it important to additionally assess this aspect.

Synthetic. Counting substructures and regressing graph topological features are notoriously hard tasks for GNNs [10, 15, 11]. We test the representational ability of `SUN` on common benchmarks of this kind [10, 11]. Table 1 reports results on the substructure counting suite, on which `SUN` attains state-of-the-art results in 3 out of 4 tasks. Additional results on the regression of global, structural properties are reported in Appendix G.

Real-world. On the molecular ZINC-12k benchmark (constrained solubility regression) [41, 19, 14], `SUN` exhibits best performance amongst all domain-agnostic GNNs under the 500k

[4] As a result, the architecture can mark root nodes, for example.



(a) (b) (c)

Figure 3: Generalisation capabilities of Subgraph GNNs in the counting prediction task (Figures 3a and 3b) and in the ZINC-12k dataset (Figure 3c).

parameter budget, including other Subgraph GNNs (see Table 1). A similar trend is observed on the large-scale Molhiv dataset from the OGB [20] (inhibition of HIV replication). Results are in Table 2. Remarkably, on both datasets, `SUN` either outperforms or approaches HIMP [16], GSN [9] and CIN [7], GNNs which explicitly model rings. We experiment on smaller-scale TUDatasets [32] in Appendix G, where we also compare selection policies.

Generalisation from limited data. In this set of experiments we compare the test performance of Subgraph GNNs when trained on increasing fractions of the available training data. Each architecture is selected by tuning the hyperparameters on the entire training and validation sets. We run this experiment on the 4-cycle counting task and the real-world ZINC-12k. We illustrate results in Figures 3a to 3c. Except for a short initial phase in the EGO policy, `SUN` generalises better than other Subgraph GNNs on cycle-counting. On ZINC-12k, `SUN` outruns DSS-, DS-GNN and GNN-AK variants from, respectively, 20, 30 and 40% of the samples. These results demonstrate that `SUN`'s expressiveness is not at the expense of sample efficiency, suggesting that its modelled symmetries guarantee strong representational power while retaining important inductive biases for learning on graphs.

Table 2: Test results for OGB dataset. GIN base-encoder for each Subgraph GNN.

Method	OGBG-MOLHIV **ROC-AUC (%)**
GCN [23]	76.06±0.97
GIN [45]	75.58±1.40
PNA [11]	79.05±1.32
DGN [5]	79.70±0.97
HIMP [16]	78.80±0.82
GSN [9]	80.39±0.90
CIN [7]	**80.94**±0.57
Reconstr.GNN [12]	76.32±1.40
DS-GNN (EGO+) [6]	77.40±2.19
DSS-GNN (EGO+) [6]	76.78±1.66
GNN-AK+ [50]	79.61±1.19
SUN (EGO+)	80.03±0.55

8 Conclusions

Our work unifies, extends, and analyses the emerging class of Subgraph GNNs. Notably, we demonstrated that the expressive power of these methods is bounded by `3-WL`. Towards a systematic study of models whose expressivity lies between `1-` and `3-WL`, we proposed a new family of layers for the class of Subgraph GNNs and, unlike most previous works on the expressive power of GNNs, we also investigated the generalisation abilities of these models, for which `SUN` shows considerable improvement. Appendix E lists several directions for future work, including an extension of our work to higher-order node-based policies.

Societal impact. We do not envision any negative, immediate societal impact originating from our theoretical results, which represent most of our contribution. Experimentally, our model has shown promising results on molecular property prediction tasks and strong generalisation ability in low-data regimes. This leads us to believe our work may contribute to positively impactful pharmaceutical research, such as drug discovery [17, 3].

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] We discussed limitations of several previous works, as well as our own model, throughout the paper as our main contribution.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Section 8.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendices B and D.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Appendix G.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Appendix G.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We report the standard deviation computed over multiple seeds for experiments on ZINC12k (Table 1), ogbg-molhiv (Table 2) and on all generalisation experiments (Figures 3a to 3c). We report the standard deviation for the "Counting Substructures" experiments (Table 1) in Appendix G.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Appendix G.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
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(d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]

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5. If you used crowdsourcing or conducted research with human subjects...

(a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]