Building powerful and equivariant graph neural networks with structural message-passing

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Abstract

Message-passing has proved to be an effective way to design graph neural networks, as it is able to leverage both permutation equivariance and an inductive bias towards learning local structures to achieve good generalization. However, current message-passing architectures have a limited representation power and fail to learn basic topological properties of graphs. We address this problem and propose a new message-passing framework that is powerful while preserving permutation equivariance. Specifically, we propagate unique node identifiers in the form of a one-hot encoding in order to learn a local context matrix around each node. This enables to learn rich local information about both features and topology, which can be pooled to obtain node representations. Experimentally, we find our model to be superior at predicting various graph topological properties, opening the way to novel powerful architectures that are both equivariant and computationally efficient.

1 Introduction

Graph neural networks have recently emerged as a popular way to process and analyze graph-structured data. Among the numerous architectures that have been proposed, the class of message-passing neural networks (MPNNs) [1–3] has been by far the most widely adopted. In addition to being able to efficiently exploit the sparsity of graphs, MPNNs exhibit an inherent tendency towards learning relationships between nearby nodes. This inductive bias is generally considered as a good fit for problems that require relational reasoning [4], such as tractable relational inference [5, 6], problems in combinatorial optimization [7–10] or the simulation of physical interactions between objects [11, 12].

A second key factor to the success of MPNNs is their equivariance properties. Since neural networks can ultimately only process tensors, in order to use a graph as input, it is necessary to order its nodes and build an adjacency list or matrix. Non-equivariant networks tend to exhibit poor sample efficiency as they need to explicitly learn that all representations of a graph in the (enormous) symmetry group of possible orderings actually correspond to the same object. On the contrary, permutation equivariant networks, such as MPNNs, are better equipped to generalize as they already implement the prior knowledge that any ordering is arbitrary.

Despite their success, equivariant MPNNs possess limited expressive power [13, 14]. For example, they cannot learn whether a graph is connected, what is the local clustering coefficient of a node, or if a given pattern such as a cycle is present in a graph [15]. For tasks where the graph structure is important, such as the prediction of chemical properties of molecules [16, 17] and the solution to combinatorial optimization problems, more powerful graph neural networks are necessary.

Aiming to address these challenges, this work puts forth structural message-passing (SMP)—a new type of graph neural network that is significantly more powerful than MPNNs, while also sharing the...
We further show in a multitask setting [21] that SMP clearly outperforms powerful message-passing networks that are not equivariant (due to their use of random node identifiers). Overall, these results show that SMP is able to overcome a major limitation of MPNNs, validating the pertinence and potential of powerful and equivariant architectures within the message-passing framework.

Concretely, SMP maintains at each node a matrix called “local context” (instead of a feature vector as in MPNNs) that is using a one-hot encoding of the nodes and the node features. These local contexts are then propagated in such a way that a permutation of the nodes will reorder the lines of each context without changing their content, thus preserving equivariance.

We evaluate SMP on a diverse set of structural tasks that are known to be difficult for message-passing architectures, such as cycle detection, connectivity testing, diameter and shortest path distance computation. In all cases, our approach compares favorably to previous methods: SMP solves cycle detection in all evaluated configurations, whereas provably powerful graph networks (PPGNs) [20] struggle when the graphs become larger, and MPNNs do not manage to solve the task completely. We further show in a multitask setting [21] that SMP clearly outperforms powerful message-passing networks that are not equivariant (due to their use of random node identifiers). Overall, these results show that SMP is able to overcome a major limitation of MPNNs, validating the pertinence and potential of powerful and equivariant architectures within the message-passing framework.

Notation. In the following, we consider the problem of representation learning on one or several graphs of possibly varying sizes. Each graph \( G = (V, E) \) has an adjacency matrix \( A \in \mathbb{R}^{n \times n} \), and potentially node attributes \( X = (x_1, \ldots, x_n)^T \in \mathbb{R}^{n \times c_X} \) and edge attributes \( y_{ij} \in \mathbb{R}^{c_Y} \) for every \((v_i, v_j) \in E\). These attributes are aggregated into a 3-d tensor \( Y \in \mathbb{R}^{n \times n \times c_Y} \). We consider the edge weights of weighted graphs as edge attributes and view \( A \) as a binary adjacency matrix. The set of neighbors of a node \( v_i \in V \) is written as \( N_i \).

2 Related work

2.1 Permutation equivariant graph neural networks

Originally introduced by Scarselli et al. [1], MPPNs have progressively been extended to handle edge attributes and graph-level attributes [3]. Despite the flexibility in their parametrization, MPNNs without special node attributes all have limited expressive power, even in the limit of infinite depth and width. For instance, they are at most as good at isomorphism testing as the Weisfeiler-Lehman (WL) vertex refinement algorithm [22][13]. The WL test has higher dimensional counterparts (k-WL) of increasing power, which has motivated the introduction of the more powerful k-WL networks [14]. However, these higher-order networks are global, in the sense that they iteratively update the state of a k-tuple of nodes based on all other k-tuples (and not only neighbours), a procedure which is very costly both in time and memory.

Recent studies have also characterized the expressive power of MPNNs from other perspectives, such as the ability to approximate continuous functions on graphs [23] and solutions to combinatorial problems [24], highlighting similar limitations of MPNNs — see also [25][29].

Beyond message-passing architectures, there have been efforts to construct more powerful equivariant networks. These networks are built by arranging together a set of simple permutation equivariant functions and operators, which are:

- Linear equivariant functions between tensors of arbitrary orders: a basis for these functions was computed by Maron et al. [30], by solving the linear system imposed by equivariance.
- Element-wise functions, applied independently to each feature of a tensor.
- Operators that preserve equivariance, such as +, -, tensor and elementwise products, composition and concatenation along the dimension of the channels.

Similarly to Morris et al. [14], networks built this way obtain a better expressive power than MPNN by using higher-order tensors [31][50]. Since k-th order tensors can represent any k-tuple of nodes, architectures manipulating them can exploit more information to compute topological properties (and be as powerful as the k-WL test). Unfortunately, memory requirements are exponential in the tensor order, which makes these methods of little practical interest. More recently, Maron et al. [20] proposed provably powerful graph networks (PPGN) based on the observation that the use of matrix
In the SMP model, each local context $U_i^{(l)}$ is an $n \times c_l$ matrix, with each row storing the $c_l$-dimensional representation of a node (denoted by color). The figure shows the local context in the output of the first layer and blank lines correspond to nodes that have not been encountered yet. Upon node reordering, the lines of the local context are permuted but their content remains unchanged.

multiplication can make their model more expressive for the same tensor order. Key differences between PPGN and our method are that (i) SMP can be parametrized to have a lower time complexity, due to the ability of message-passing to exploit the sparsity of adjacency matrices, (ii) SMP retains the message-passing inductive bias, which is different from PPGN and, as we will show empirically, makes it better suited to practical tasks such as the detection of substructures in a graph.

2.2 Non-equivariant graph neural networks

In order to better understand the limitations of current graph neural networks, analogies with graph theory and distributed systems have been exploited. In particular, a large class of problems in these fields cannot be solved without using node identifiers [32, 33]. The reasoning is that, in message-passing architectures, each node has access to a local view of the graph created by the reception of messages. Without identifiers, each node can count the number of incoming messages and process them, but cannot tell from how many unique nodes they come from. They are therefore unable to reconstruct the graph topology.

This observation has motivated researchers to provide nodes with randomly selected identifiers [18, 19, 34, 35]. Encouragingly, by showing the equivalence between message-passing and a model in distributed algorithms, Loukas [19] proved that graph neural networks with identifiers and sufficiently expressive message and update functions can be Turing universal, which was also confirmed on small instances of the graph isomorphism problem [36].

Nevertheless, the main issue with these approaches is sample efficiency. Identifiers introduce a dependency of the network to a random input and the loss of permutation equivariance, causing poor generalization. Although empirical evidence has been presented that the aforementioned dependency can be overcome with large amounts of training data or other augmentations [18, 36], overfitting and optimization issues can occur. In this work, we propose to overcome this problem by introducing a network which is both powerful and permutation equivariant.

3 Structural message-passing

We present here the structural message-passing neural networks (SMP), which is a generalization of MPNNs that processes node identifiers in an equivariant manner. Our idea is simple: rather than relying only on permutation invariant embeddings or on non-equivariant identifiers (as in recent universal models), the state of every node in SMP depends on changes in the node ordering in an equivariant manner.

3.1 Method

In SMP, each node of a graph maintains a local context matrix $U_i \in \mathbb{R}^{n \times c}$ rather than a feature vector $x_i \in \mathbb{R}^c$ as in MPNN. The $j$-th row of $U_i$ contains the $c$-dimensional representation that node $v_i$ has of node $v_j$. Intuitively, equivariance means that the lines of the local context are simply permuted if the nodes are reordered, as shown in Fig. 1.
**Initialization**  The local context is initialized as a one-hot encoding \(U_i^{(0)} = \mathbb{1}_i \in \mathbb{R}^{n \times 1}\) for every \(v_i \in V\), which corresponds to having initially a unique identifier for each node. In addition, if there are features \(x_i\) associated with node \(v_i\), they are appended to the same row of the local context as the identifiers: \(U_i^{(0)}[i, :] = [1, x_i] \in \mathbb{R}^{c \times 1}\).

**Layers**  At layer \(l + 1\), the state of each node is updated as in standard MPNNs [3]: messages are computed on each edge before being aggregated into a single matrix via a symmetric function. The result can then be updated using the local context of previous layer at this node:

\[
U_i^{(l+1)} = u^{(l)}\left(U_i^{(l)}, \hat{U}_i^{(l)}\right) \in \mathbb{R}^{n \times c_{l+1}} \quad \text{with} \quad \hat{U}_i^{(l)} = \phi\left(m^{(l)}\left(U_i^{(l)}, U_j^{(l)}, y_j\right)_{v_j \in N_i}\right)
\]

Above, \(u^{(l)}, m^{(l)}, \phi\) are the update, message and aggregation functions of the \((l + 1)\)-th layer, respectively, whereas \(c_{l+1}\) denotes the layer’s width. Interestingly, in the simple case where a one-hot encoding of the nodes is propagated using \(U_i^{(l+1)} = \sum_{v_j \in N_i} U_j^{(l)}\), powers of the adjacency matrix are obtained. As \(A[l, i, j]\) corresponds to the count of walks of length \(l\) between \(v_i\) and \(v_j\), there is a natural connection between the propagation of identifiers and the detection of topological features.

In the following, it will be convenient to express each SMP layer \(f^{(l)}\) in a tensor form:

\[
U^{(l+1)} = f^{(l)}(U^{(l)}, Y, A) = [U_1^{(l+1)}, \ldots, U_n^{(l+1)}] \in \mathbb{R}^{n \times n \times c_{l+1}}
\]

**Pooling**  After all \(L\) message-passing layers have been applied, the aggregated contexts \(U^{(L)}\) can be pooled to a vector or to a matrix (e.g. for graph and node classification, respectively). To obtain an equivariant representation, we aggregate each \(U_i^{(L)} \in \mathbb{R}^{n \times c_L}\) into a vector using an equivariant neural network for sets \(\mathbb{S}_n\) [37-40] applied simultaneously to each node \(v_i\):

\[
f_{eq}(U^{(0)}, Y, A) = \sigma \circ f^{(L)} \circ \cdots \circ f^{(1)}(U^{(0)}, Y, A) \in \mathbb{R}^{n \times c},
\]

whereas a permutation invariant representation is obtained after the application of a pooling function \(pool\). It may be a simple sum or average followed by a soft-max, or a more complex operator [41]:

\[
f_{im}(U^{(0)}, Y, A) = pool \circ f_{eq}(U^{(0)}, Y, A) \in \mathbb{R}^{c}
\]

### 3.2 Analysis

The following section characterizes the equivariance properties and representation power of SMP. For the sake of clarity, we defer all proofs to the appendix.

**Equivariance**  Before providing sufficient conditions for permutation equivariance, we define it formally. A change in the ordering of \(n\) nodes can be described by a permutation \(\pi\) of the symmetric group \(\mathbb{S}_n\), \(\pi\) acts on a tensor by permuting the axes indexing nodes (but not the other axes):

\[
(\pi \cdot U)[i, j, k] = U[\pi^{-1}(i), \pi^{-1}(j), k], \quad \text{where} \quad U \in \mathbb{R}^{n \times n \times c}
\]

For vector and matrices, the action of a permutation is more easily described using the matrix \(\Pi\) canonically associated to \(\pi\): \(\pi.z = z\) for \(z \in \mathbb{R}^c\), \(\pi.X = \Pi^T X\) for \(X \in \mathbb{R}^{n \times c}\), and \(\pi.A = \Pi^T A \Pi\) for \(A \in \mathbb{R}^{n \times n}\). An SMP layer \(f\) is said to be permutation equivariant if permuting the inputs and applying \(f\) is equivalent to first applying \(f\) and then permuting the result:

\[
\forall \pi \in \mathbb{S}_n, \quad \pi \cdot f(U, Y, A) = f(\pi.U, \pi.Y, \pi.A)
\]

We can now state some sufficient conditions for equivariance:

**Theorem 1 (Permutation equivariance).** Let functions \(m, \phi\) and \(u\) be permutation equivariant, that is, for every \(\pi \in \Pi\) we have \(u(\pi.U, \pi.U') = \pi.u(U, U')\), \(\phi(\{\pi.U\}_v \in N_i) = \pi.\phi(\{U\}_v \in N_i)\), and \(m(\pi.U, \pi.U', y) = \pi.m(U, U', y)\). Then, SMP is permutation equivariant.

The proof is presented in Appendix A. This theorem defines the class of functions that can be used in our model. For example, if the message and update functions are operators applied simultaneously to each row of the local context, the whole layer is guaranteed to be equivariant. However, more general functions can be used: each \(U_j\) is a \(n \times c\) matrix which can be viewed as the representation of a set of nodes. Hence, any equivariant neural network for sets can be used. Importantly, as neural networks for sets are able to take sets of different sizes as input, it is the case of SMP as well: as the number of rows in each local context has no influence on the parametrization, our method can be trained with graphs of different sizes.
Representation and expressive power  The following theorem characterizes the representation power of SMP when parametrized with powerful layers. For simplicity, we consider unattributed graphs. We also ease notation by omitting the $U^{(l)}$ argument of SMP. Simply put, Theorem 2 asserts that it is possible to parameterize an SMP network such that it maps non-isomorphic graphs to different representations:

**Theorem 2 (Representation power).** Consider the class of simple graphs of diameter at most $\Delta$ and degree at most $d_{\text{max}}$. There exists a permutation equivariant SMP network $f : \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n \times c}$ of depth at most $\Delta$ and width at most $2d_{\text{max}}$ such that, for any two graphs $G$ and $G'$ with respective adjacency matrices $A$ and $A'$, the following statements hold for every $v_i \in V$ and $v_j \in V'$:

- If $G$ and $G'$ are not isomorphic, then $\Pi^T f(A)[i, :, :] \neq f(A')[j, :, :]$ for all $\pi \in \mathfrak{S}_n$.
- If $G$ and $G'$ are isomorphic, then $\Pi^T f(A)[i, :, :] = f(A')[j, :, :]$ for some $\pi \in \mathfrak{S}_n$.

The proof is detailed in Appendix [B]. We first show the result for the simple case where each $U_i$ is a $n \times n$ matrix, and then consider the case of $n \times 2d_{\text{max}}$ matrices using the following lemma:

**Lemma 1 (Maehara and Rödl [42]).** For any simple graph $G = (V, E)$ of $n$ nodes and maximum degree $d_{\text{max}}$, there exists a unit-norm embedding of the nodes $X \in \mathbb{R}^{n \times 2d_{\text{max}}}$ such that for every $v_i, v_j \in V$, $(v_i, v_j) \in E \iff X_i \perp X_j$.

The universality of SMP is a direct corollary: since each node has the ability to uniquely represent the adjacency matrix of its input graph as a set, it can also employ a universal network for sets [37] to compute any equivariant function on the graph (cf. Appendix [C]).

**Corollary 1 (Expressive power).** Let $G$ be a simple graph of diameter at most $\Delta$ and degree at most $d_{\text{max}}$. Consider an SMP $f = f^{(L)} \circ \cdots \circ f^{(1)}$ of depth $L = \Delta$ and width $2d_{\text{max}}$ satisfying the properties of Theorem 2. Then, any equivariant function can be computed as $f_{\text{eq}} = \sigma \circ f$, where $\sigma$ is a universal function of sets applied simultaneously to each node. Similarly, any permutation invariant function can be computed as $f_{\text{in}} = \frac{1}{n} \sum_{v_i \in V} \sigma \circ f$.

We note that the proofs of Theorem 2 and Corollary 1 are not constructive and rely on the SMP being built out of powerful layers that may deviate from practical implementations. Deriving a universality result for practical layer parameterizations remains an open question. Nevertheless, we do constructively prove the following more straightforward claim using a practical parametrization:

**Proposition 1.** SMP is strictly more powerful than MPNN: SMP can simulate any MPNN with the same number of layers, but MPNNs cannot simulate all SMPs.

To prove it, we create for any MPNN a corresponding SMP which performs the same operations as the MPNN on the main diagonal of the local context. On the contrary, we can easily create an SMP which is able to distinguish between two small graphs that cannot be distinguished by the Weisfeiler-Lehman test (Appendix [D]).

4 Implementation

SMP offers a lot of flexibility in its implementation. This section describes two specific parametrizations (one faster and the other more expressive) that we found to work well in practice, but our framework can also be implemented differently.

Default SMP  In SMP, a message function combines the local context of a pair of nodes and any edge feature vector in an equivariant manner. In our default parametrization, the operation of the message function $m_{\text{def}}^{(l)}$ is split in two steps. The first one modifies the local context at each node $v_i$ in $V$ using a subset of the linear equivariant functions computed by Maron et al. [30]:

$$
\hat{U}_i^{(l)} = U_i^{(l)} W_1^{(l)} + \frac{1}{n} I_n^T U_i^{(l)} W_2^{(l)} + 1_n (c^{(l)})^T + \frac{1}{n} I_n^T U_i^{(l)} W_3^{(l)},
$$

where $1_n \in \mathbb{R}^{n \times 1}$ is a vector of ones, $I_n \in \mathbb{R}^{n \times 1}$ the indicator of $v_i$, whereas $(W_k^{(l)})_{1 \leq k \leq 5}$ and $c^{(l)}$ are learnable parameters. The second step is the computation of the messages, equal to

$$
m_{\text{def}}^{(l)}(\hat{U}_i^{(l)}, \hat{U}_j^{(l)}, y_{ij}) = \hat{U}_j^{(l)} + \text{ReLU}(\|\hat{U}_i^{(l)}\|_{1} \|\hat{U}_j^{(l)}\|_{2} y_{ij}^{(l)} W_4^{(l)} W_5^{(l)}),
$$

(1)
An apparent drawback of SMP (shared by all equivariant powerful architectures we are aware of) is while also avoiding the exploding-norm problem [43].

\[ \parallel \] denotes the concatenation along the second axis. This function adds to \( \hat{U}_j^{(l)} \) a term that is meant to measure the similarity between local contexts. Finally, the \( l \)-th SMP layer returns

\[
U_i^{(l+1)} = \frac{1}{d_{\text{avg}}} \sum_{v_j \in N_i} m_{\text{def}}^{(l)}(U_i^{(l)}, U_j^{(l)}, y_{ij}),
\]

with the average degree \( d_{\text{avg}} \) normalization retaining the good properties of the sum aggregator [13], while also avoiding the exploding-norm problem [43].

**Fast SMP** We also propose a second parametrization for graphs without edge features. In Fast SMP, the local contexts are first updated in the same way, but the two-layer network of the message function (1) is replaced by a pointwise multiplication \( \odot \), as:

\[
m_{\text{fast}}^{(l)}(\hat{U}_i^{(l)}, \hat{U}_j^{(l)}) = \hat{U}_j^{(l)} + \left( \hat{U}_i^{(l)} W_4^{(l)} \odot \hat{U}_j^{(l)} W_5^{(l)} \right),
\]

so that the \( l \)-th SMP layer updates each node’s local context as

\[
U_i^{(l+1)} = \frac{1}{d_{\text{avg}}} \sum_{v_j \in N_i} m_{\text{fast}}^{(l)}(U_i^{(l)}, U_j^{(l)}) = \frac{1}{d_{\text{avg}}} \left( \sum_{v_j \in N_i} \hat{U}_j^{(l)} + \hat{U}_i^{(l)} W_4^{(l)} \odot \sum_{v_j \in N_i} \hat{U}_j^{(l)} W_5^{(l)} \right).
\]

On the r.h.s. of the last equation, the arguments of the two sums are only functions of the local context of node \( v_j \). This allows for a more efficient implementation, where one message is computed per node, instead of one per edge as in default SMP.

One might notice that Fast SMP can be seen as a local version of PPGN (Appendix [F]).

**Proposition 2.** A Fast SMP with \( k \) layers can be approximated by a 2\( k \)-block PPGN.

Being local makes SMP more computationally efficient. Furthermore, as we will see experimentally, SMP manages to learn topological information much more easily than PPGN, a property that we attribute to the inductive bias carried by message-passing.

**Complexity** Table [1] compares the per-layer space and time complexity induced by the forward pass of SMP with that of other standard graph networks. Whereas local order-3 Weisfeiler-Lehman networks need to store all triplets of nodes, both PPGN and SMP only store information for pairs of nodes. However, message-passing architectures (such as SMP) can leverage the sparsity of the adjacency matrix and hence benefit from a more favorable time complexity than architectures which perform global updates (as PPGN).

An apparent drawback of SMP (shared by all equivariant powerful architectures we are aware of) is the need for more memory than MPNN. This difference is partially misleading since it is known that the width of any MPNN needs to grow at least linearly with \( n \) (for any constant depth) for it to be able to solve many graph-theoretic problems [19] [21] [36]. However, for graphs with a large diameter, the memory requirements of SMP can be relaxed by using the following observation: if each node is colored differently from all nodes in its 2\( k \)-hop neighborhood, then no node will see the same color twice in its \( k \)-hop neighborhood. It implies that nodes which are far apart can use the same identifier.

**Table 1:** Time and space complexity of the forward pass expressed in terms of number of nodes \( n \), number of edges \( m \), number of node colors \( \chi \), and width \( c \). For connected graphs, we trivially have \( \chi \leq n \leq m + 1 \leq n^2 \).

| Method               | Memory per layer | Time complexity per layer |
|----------------------|------------------|---------------------------|
| GIN [13]             | \( \Theta(nc) \)  | \( \Theta(mc + nc^2) \)   |
| MPNN [2]             | \( \Theta(nc) \)  | \( \Theta(mc^2) \)        |
| Fast SMP (with coloring) | \( \Theta(nc\chi) \) | \( \Theta(m\chi c + n\chi c^2) \) |
| Fast SMP             | \( \Theta(n^2c) \) | \( \Theta(mn c + n^2c^2) \) |
| SMP                  | \( \Theta(n^2c) \) | \( \Theta(mn c^2) \)       |
| PPGN [20]            | \( \Theta(n^2c) \) | \( \Theta(n^3c + n^2c^2) \) |
| Local order-3 WL [14] | \( \Theta(n^4c) \) | \( \Theta(n^4c + n^3c^2) \) |
Figure 2: (left) Architecture for cycle detection. The graph extractor computes the trace and the sum along the two first axes of $U$, and passes the result into a two-layer MLP in order to produce a set of global features. (right) Architecture for multi-task learning: after each convolution, node features are extracted using a two-layer MLP followed by three pooling methods (mean, max, and the extraction of $U[i,i,:]$ for each $v_i \in V$), and a final linear layer. The rest of the architecture is similar to Corso et al. [21]: it uses a Gated Recurrent Unit (GRU) and a Set-to-set network (S2S).

Figure 3: Test accuracy on the detection of cycles of various length. (Best seen in color.) Despite the large amount of train data, only SMP is able to solve the problem in all configurations.

Table 2: Test accuracy (%) on the detection of 6 cycles for graphs with 56 nodes.

| Train samples | 200  | 500  | 1000 | 5000 |
|---------------|------|------|------|------|
| GIN random id | 65.8 | 70.8 | 80.6 | 96.4 |
| SMP           | 87.7 | 97.4 | 97.6 | 99.5 |

5 Experiments

We evaluate the performance of our method on several tasks related to the detection of structural graph properties.

5.1 Cycle detection

We first evaluate different architectures on the detection of cycles of length 4, 6 and 8. Models are implemented with Pytorch Geometric [44], retrained for each cycle length and graph size on 10k samples with balanced classes, and evaluated on 10,000 samples as well. All models follow the same jumping knowledge structure [45] shown on Fig. 2, as it performed much better on this task than the original architectures for GIN [13] and PPGN. As a result, the methods under comparison only differ in the definition of the convolution, making comparison easy. We use Fast SMP, as we find its expressivity to be sufficient for this task.

Results are shown in Fig 3. For a given cycle length, the task becomes harder as the number of nodes in the graph grows: the bigger the graph, the more candidate paths that the network needs to verify.

Source code is available at https://github.com/cvignac/SMP
We introduced structural message-passing (SMP), a new architecture that is both powerful and permutation equivariant, solving a major weakness of previous message-passing networks. Empirically, SMP significantly outperforms previous models in learning graph topological properties. We believe that our work paves the way to graph neural networks that efficiently manipulate both node and topological features, with potential applications to chemistry, computational biology and neural algorithmic reasoning.

5.2 Multi-task detection of graph properties

We further benchmark SMP on the multi-task detection of graph properties proposed in Corso et al.\cite{corso2020equivariant}. The goal is to estimate three node-defined targets: geodesic distance from a given node (Dist.), node eccentricity (Ecc.), and computation of Laplacian features $Lx$ given a vector $x$ (Lap.), as well as three graph-defined targets: connectivity (Conn.), graph diameter (Diam.), and spectral radius (Rad.). The training set is composed of 5120 graphs with up to 24 nodes, while graphs in the test set have up to 19 nodes. Several MPNNs are evaluated as well as PNA\cite{henaff2019data}, a message-passing model based on the combination of several aggregators. Importantly, random identifiers are used for all these models, so that the main difference with SMP is their lack of permutation equivariance.

All models are benchmarked using the same architecture, apart from the fact that SMP manipulates local contexts. In order to pool these contexts into node features and use them as input to the Gated Recurrent Unit\cite{cho2014properties}, we use an extractor described in Figure\cite{fig:extraction}. As an ablation study, we also consider for each model a corresponding MPNN with the same architecture, except that it manipulates node features instead of the local contexts (and therefore does not use the extractor either).

The results are summarized in Table\cite{table:multi-task}. We find that both SMPs are able to exploit the local contexts, as they perform much better than the corresponding MPNN. SMP also outperforms other methods by a significant margin. Lastly, standard SMP tends to achieve better results than fast SMP on tasks that require graph traversals, which may be due to a better representation power. Overall, these results show that SMPs are able to efficiently learn topological information, reaching an essential milestone towards the design of graph networks that can exploit both features and topology on complex tasks.

6 Conclusion

We introduced structural message-passing (SMP), a new architecture that is both powerful and permutation equivariant, solving a major weakness of previous message-passing networks. Empirically, SMP significantly outperforms previous models in learning graph topological properties. We believe that our work paves the way to graph neural networks that efficiently manipulate both node and topological features, with potential applications to chemistry, computational biology and neural algorithmic reasoning.

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Table 3: Log MSE on the test set (lower is better). Baseline results are from Corso et al.\cite{corso2020equivariant}.

| Model       | Average | Dist. | Ecc. | Lap. | Conn. | Diam. | Rad. |
|-------------|---------|-------|------|------|-------|-------|------|
| SMP         | −3.59   | −3.59 | −3.67| −4.27| −2.97 | −3.58 | −3.46|
| Fast SMP    | −3.30   | −3.30 | −3.30| −4.30| −3.65 | −3.82 |      |
| Fast MPNN   | −2.77   | −3.18 | −2.05| −3.27| −2.24 | −2.88 | −2.97|
| MPNN        | −2.37   | −2.47 | −1.99| −2.83| −1.61 | −2.40 | −2.93|
| MPNN (sum)  | −2.53   | −2.36 | −2.16| −2.59| −2.54 | −2.67 | −2.87|
| GIN         | −1.99   | −2.00 | −1.90| −1.60| −1.61 | −2.17 | −2.66|
| GAT         | −2.26   | −2.34 | −2.09| −1.60| −2.44 | −2.40 | −2.70|
| PNA         | −3.13   | −2.89 | −3.77| −2.61| −3.04 | −3.57 |      |
| PPGN−       | −9.99   | −3.60 | −4.30| −2.72| −3.65 | −3.82 |      |

As being cycles. SMP is able to solve the task almost perfectly for all graph and cycle sizes. As we train on many samples (thus alleviating problems due to the lack of equivariance), we observe a strong correlation between accuracy and the presence of identifiers: random identifiers and weak identifiers (a one-hot encoding of the degree) tend to perform better than the baseline GIN and MPNN. Surprisingly, PPGN solves the task for small graphs, but fails when $n$ grows. Perhaps due to a mis-aligned inductive bias, we encountered difficulties with training PPGN—with message-passing architectures could be trained more easily. We provide a more detailed comparison between SMP and PPGN in Appendix\cite{appendix}.

We also compare SMP and GIN with random identifiers in settings with less training data. Table\cite{table:random-identifiers} shows that SMP requires much fewer samples to achieve good performance, which confirms the importance of equivariance in graph neural networks.
Broader Impact

This paper introduced a new methodology for building graph neural networks, conceived independently of a specific application. As graphs constitute a very abstract way to represent data, they have found a lot of different applications \[47\]. The wide applicability of graph neural networks makes it challenging to foresee how our method will be used and the ethical problems which might occur.

Nevertheless, as we propose to overcome limitations of previous work in learning topological information, our method is likely to be used first and foremost in fields were graph topology is believed to be important. We hope in particular that it can contribute to the fields of quantum chemistry and drug discovery. Other applications come to mind: material science \[48\], computational biology \[49\], combinatorial optimization \[7–9\] or code generation \[50\].

Acknowledgments and Disclosure of Funding

Clément Vignac would like to thank the Swiss Data Science Center for supporting him through the PhD fellowship program (grant P18-11). Andreas Loukas would like to thank the Swiss National Science Foundation for supporting him in the context of the project “Deep Learning for Graph-Structured Data” (grant number PZ00P2 179981).

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A  Proof of Theorem 1

Let \( f \) be a layer of SMP:
\[
  f(U, Y, A)[i,:,:) = u(U, \phi(\{m(U, U_j, y_{ij})\}_{v_j \in N_i})) = u(U, \phi(\{m(U, U_j, y_{ij})\}_{v_j : A[i,j]<0}))
\]
The action of a permutation \( \pi \) on the inputs is defined as \( f(\pi(U, Y, A)) = f(\pi U, \pi Y, \pi A) \). In order to simplify notation, we will consider \( \pi^{-1} \) instead of \( \pi \). We have for example \( (\pi^{-1} A)[i,j] = A[i,j] \) and \( (\pi^{-1} U)[i,j,k] = U[i,j,k] \), which can be written as
\[
(\pi^{-1} U)[i,:,:) = \Pi U_{\pi_i}.
\]
As shown next, the theorem’s conditions suffice to render SMP equivariant:
\[
  f(\pi^{-1}(U, Y, A))[i,:,:) = u(\Pi U_{\pi_i}, \phi(\{m(\Pi U_{\pi_i}, \Pi U_{\pi_j}, y_{ij})\}_{v_j : A[i,j]<0}))
\]
\[
= u(\Pi U_{\pi_i}, \phi(\{m(\Pi U_{\pi_i}, \Pi U_{\pi_j}, y_{ij})\}_{v_j : A[i,j]<0}))
\]
\[
= u(\Pi U_{\pi_i}, \Pi \phi(\{m(U_{\pi_i}, U_{\pi_j}, y_{ij})\}_{v_j : A[i,j]<0}))
\]
\[
= \Pi f(U, Y, A)[\pi_i,:,:) = (\pi^{-1} f(U, Y, A))[i,:,:],
\]
which matches the definition of equivariance.

B  Proof of Theorem 2

The fact that embeddings produced by isomorphic graphs are permutations one of another is a consequence of equivariance, so we are left to prove the first point. To do so, we will first prove that there is an SMP that maps the initial one-hot encoding of each node to an embedding that allows to reconstruct the adjacency matrix. The theorem will then follow easily.

Consider a simple connected graph \( G = (V,E) \). For any layer \( l \in \mathbb{N} \) and node \( v_i \in V \), we denote by \( G^{(l)}_i = (V, E^{(l)}_i) \) the graph with node set \( V \) and edge set \( E^{(l)}_i = \{(v_p, v_q) \in E, d(v_i, v_p) \leq l, d(v_i, v_q) \leq l, d(v_i, v_p) + d(v_i, v_q) < 2l\} \). These edges correspond to the receptive field of node \( v_i \) after \( l \) layers of message-passing. We denote by \( A^{(l)}_i \) the adjacency matrix of \( G^{(l)}_i \).

B.1 Warm up: nodes manipulate \( n \times n \) matrices

To build intuition, it is useful to first consider the case where \( U_i \) are \( n \times n \) matrices (rather than \( n \times c \) as in SMP). In this setting, messages are \( n \times n \) matrices as well. If the initial state of each node \( v_i \) is its one-hop neighbourhood \( (U^{(1)}_i = A^{(1)}_i) \), then each node can easily recover the full adjacency matrix by updating its internal state as follows:
\[
U^{(l+1)}_i = \max_{v_j \in N_i \cup v_i} \{U^{(l)}_j\},
\]
where the max is taken element-wise.

Lemma 2. Recursion\([2]\) yields \( U^{(l)}_i = A^{(1)}_i \).

Proof. We prove the claim by induction. It is true by construction for \( l = 1 \). For the inductive step, suppose that \( U^{(l)}_i = A^{(1)}_i \). Then,
\[
U^{(l+1)}_i[p,q] = 1 \iff \exists v_j \in \{N_i \cup v_i\} \text{ such that } A^{(1)}_j[p,q] = 1
\]
\[
\iff (v_p, v_q) \in E \text{ and } \exists v_j \in \{N_i \cup v_i\}, d(v_j, v_p) \leq l, d(v_j, v_q) \leq l, d(v_j, v_p) + d(v_j, v_q) < 2l
\]
\[
\implies (v_p, v_q) \in E, d(v_i, v_p) \leq l + 1, d(v_i, v_q) \leq l + 1, d(v_i, v_p) + d(v_i, v_q) < 2(l+1)
\]
\[
\implies A^{(1+1)}_i[p,q] = 1
\]
Conversely, if \( A^{(1+1)}_i[p,q] = 1 \), then there exists either a path of length \( l \) of the form \((v_i, v_j, \ldots, v_p)\) or \((v_i, v_j, \ldots, v_q)\). This node \( v_j \) will satisfy \( U^{(l)}_j[p,q] = 1 \) and thus \( U^{(l+1)}_i[p,q] = 1 \).

[2]
It is an immediate consequence that, for every connected graph of diameter \( \Delta \), we have \( U_i^{(\Delta)} = A \).

B.2 SMP: nodes manipulate node embeddings

We now shift to the case of SMP. We will start by proving that we can find an \( n \times 2d_{\text{max}} \) embedding matrix (rather than \( n \times n \)) that still allows to reconstruct \( A_i^{(l)} \). For this purpose, we will use the following result:

**Lemma 3** (Maehara and Rödl [42]). For any simple graph \( G = (V, E) \) of \( n \) nodes and maximum degree \( d_{\text{max}} \), there exists a unit-norm embedding of the nodes \( X \in \mathbb{R}^{n \times 2d_{\text{max}}} \) such that

\[
\forall (v_i, v_j) \in V^2, (v_i, v_j) \in E \iff X_i \perp X_j.
\]

In the following we assume the perspective of some node \( v_i \in V \). Let \( U_i^{(l)} \in \mathbb{R}^{n \times c_l} \) be the context of \( v_i \). Further, write \( u_i^{(l)} = U_i^{(l)}[j, :] \in \mathbb{R}^{c_l} \) to denote the embedding of \( v_j \) at layer \( l \) from the perspective of \( v_i \). Note that, for simplicity, the index \( i \) is omitted.

**Lemma 4.** There exists a sequence \( (f_l)_{l \geq 1} \) of permutation equivariant SMP layers defining \( U_i^{(l+1)} = f^{(l+1)}(U_i^{(l)}, \{ U_j^{(l)} \}_{j \in N_i}) \) such that \( u_i^{(l)} \perp u_k^{(l)} \iff (v_j, v_k) \in E_i^{(l)} \) for every layer \( l \) and nodes \( v_j, v_k \in V \). These functions do not depend on the choice of \( v_i \in V \).

*Proof.* We use an inductive argument. An initialization (layer \( l = 1 \)), we have \( U_j^{(0)} = \delta_j \) for every \( v_j \). We need to prove that there exists \( U_i^{(l)} = f^{(l)}(U_i^{(0)}, \{ U_j^{(0)} \}_{j \in N_i}) \) which satisfies

\[
\forall (v_j, v_k) \in V^2, u_j^{(l)} \perp u_k^{(l)} \iff (v_j, v_k) \in E_i^{(l)}.
\]

Rewritten in matrix form, it is sufficient to show that there exists \( U_i^{(1)} \) such that \( U_i^{(1)}(U_i^{(1)})^T = 11^T - A_i^{(1)} \), with \( 1 \) being the all-ones vector. \( A_i^{(1)} \) is the adjacency matrix of a star consisting of \( v_i \) at the center and all its \( d_i \) neighbors at the spokes. Further, it can be constructed in an equivariant manner from the layer’s input as follows:

\[
A_i^{(1)} = \sum_{v_j \in N_i} \delta_j \delta_j^T + \sum_{v_j \in N_i} \delta_j \delta_j^T.
\]

Since the rank of \( A_i^{(1)} \) is at most \( d_i \) (there are \( d_i \) non-zero rows), the rank of \( 11^T - A_i^{(1)} \) is at most \( d_i + 1 \leq 2d_i \leq 2d_{\text{max}} \). It directly follows that there exists a matrix \( U_i^{(1)} \) of dimension \( n \times 2d_{\text{max}} \) which satisfies \( U_i^{(1)}(U_i^{(1)})^T = 11^T - A_i^{(1)} \). Further, as the construction of this matrix is based on the eigendecomposition of \( A_i^{(1)} \), it is permutation equivariant as desired.

**Inductive step.** According to the inductive hypothesis, we suppose that:

\[
u_j^{(l)} \perp u_k^{(l)} \iff (v_j, v_k) \in E_i^{(l)} \quad \text{for all} \; v_j, v_k \in V
\]

The function \( f^{(l+1)} \) builds the embedding \( U_i^{(l+1)} \) from \( (U_i^{(l)}, \{ U_j^{(l)} \}_{j \in N_i}) \) in three steps:

**Step 1.** Each node \( v_j \in N_i \) sends its embedding \( U_j^{(l)} \) to node \( v_i \). This is done using the message function \( m^{(l)} \).

**Step 2.** The aggregation function \( \phi \) reconstructs the adjacency matrix \( A_j^{(l)} \) of \( G_j^{(l)} \) from \( U_j^{(l)} \) for each \( v_j \in N_i \cup \{ v_i \} \). This is done by testing orthogonality conditions, which is a permutation equivariant operation. Then, it computes \( A_i^{(l+1)} \) as in Lemma 2 using

\[
A_i^{(l+1)} = \max \{(A_j^{(l+1)})_{v_j \in N_i \cup \{ v_i \}}\},
\]

with the maximum taken entry-wise.

**Step 3.** The update function \( u^{(l)} \) constructs an embedding matrix \( U_i^{(l+1)} \in \mathbb{R}^{n \times 2d_{\text{max}}} \) that allows to reconstruct \( A_i^{(l+1)} \) through orthogonality conditions. The existence of such an embedding is guaranteed by Lemma 1. This operation can be performed in a permutation equivariant manner by ensuring that the order of the rows of \( U_i^{(l+1)} \) is identical with that of \( A_i^{(l+1)} \).
Therefore, the constructed embedding matrix $U^{(l+1)}_i$ satisfies
\[
u^{(l+1)}_j \perp u^{(l+1)}_k \iff (v_j, v_k) \in E^{(l+1)}_i \text{ for all } v_j, v_k \in V
\]
and the function $f^{(l+1)}$ is permutation equivariant (as a composition of equivariant functions).

It is a direct corollary of Lemma 1 that, when the depth is at least as large as the graph diameter, such that $E^{(l)}_i = E$ for all $v_i$ and the width is at least as large as $2d_{\text{max}}$, then there exist a permutation equivariant SMP $f = f^{(L)} \circ \ldots \circ f^{(1)}$ that induces an injective mapping from the adjacency matrix $A$ to the local context $U_i$ of each node $v_i$. As a result, given two graphs $G$ and $G'$, if there are two nodes $v_i \in V$ and $v_j' \in V'$ and a permutation $\pi \in S_n$ such that $U^{(L)}_i = \Pi U^{(L)}_{j'}$, then the orthogonality conditions will yield $A = \Pi^T A' \Pi$. The contraposition is that if two nodes belong to graphs that are not isomorphic, their embedding will belong to two different equivalence classes (i.e. they will be different even up to permutations).

We have shown that there exists an SMP that satisfies the conditions of the theorem, and specifically, we demonstrated the each layer can be decomposed in a message, aggregation and update functions exactly.

The main assumption of our proof is that the aggregation and update functions can exactly compute any function of their input — this is impossible in practice. An extension of our argument to a universal approximation statement would entail substituting the aggregation and update functions by appropriate universal approximators. In particular, the aggregation function manipulates a set of $n \times n$ matrices, which can be represented as a $n \times n \times c$ tensor with some lines zeroed out. Some universal approximators of equivariant functions for these tensors are known [51], but they have large memory requirements. Therefore, proving that a given parametrization of an SMP can be used to approximately reconstruct the adjacency matrix hinges on the identification of a simple universal approximator of equivariant functions on $n \times n \times c$ tensors.

### C Proof of Corollary 1

Lemma 1 proves the existence of an injective mapping from adjacency matrices of simple graphs to features for a set of nodes. Therefore, any permutation equivariant function $h_{\text{eq}}(A)$ on adjacency matrices can be expressed by an equivariant function on sets
\[
h_{\text{eq}}(A) = h'_{\text{eq}}(U) \quad \text{with} \quad U[i,:) = u_i \in \mathbb{R}^{2d_{\text{max}}} \quad \forall v_i \in V,
\]
as long as the node embeddings $u_1, \ldots, u_n$ allow the reconstruction of $A$, e.g., through orthogonality conditions. It was proven in Theorem 2 that, under the corollary’s conditions, the local context $U^{(L)}_i$ of any node $v_i$ yields an appropriate matrix $U$. In order to compute $h_{\text{eq}}$, each node can then rely on the universal $\sigma$ to compute the invariant function:
\[
h_{\text{inv}}^{(l)}(U, 1_i) = h'_{\text{eq}}(U)[i,:) = h_{\text{eq}}(A)[i,:] \in \mathbb{R}^c.
\]

For invariant functions $h_{\text{inv}}(A) \in \mathbb{R}^c$, it suffices to build the equivariant function $h_{\text{eq}}(A) = [h_{\text{inv}}(A), \ldots, h_{\text{inv}}(A)] \in \mathbb{R}^{n \times c}$. Then, if each node $v_i$ computes $h_{\text{eq}}(A)[i,:]=h_{\text{inv}}(A)$, averaging will yield $\frac{1}{n} \sum_{v_i \in V} h_{\text{eq}}(A)[i,:] = h_{\text{inv}}(A)$, as required.

### D Proof of Proposition 1

SMPs are at least as powerful as MPNNs We will show by induction that any MPNN can be simulated by an SMP:

**Lemma 5.** For any MPNN mapping initial node features $(x^{(0)}_i)_{v_i \in V}$ to $(x^{(L)}_i)_{v_i \in V}$, there is an SMP with the same number of layers such that
\[
\forall v_i \in V, \forall l \leq L, \quad U^{(l)}[i,i,:] = x^{(l)}_i \quad \text{and} \quad \forall j \neq i, \quad U^{(l)}[i,j,:] = 0.
\]
Weisfeiler-Lehman test or by MPNNs without special node features [20]. On the contrary, consider as any MPNN can be computed by an SMP, we conclude that SMPs are at least as powerful as

\[ G \]

To do so, we propose to build a graph

\[ \widetilde{G} \]

where

\[ \tilde{\Delta} \]

In SMP, the initial local context is a one-hot encoding of each node:

\[ \tilde{U} \]

and the following SMP layer:

\[ \tilde{U}^{(l+1)} = \text{diag}(\hat{\mu}(\tilde{U}^{(l)}), \tilde{\phi}(\{ \tilde{m}(\tilde{U}^{(l)}), \tilde{U}^{(l)}, \tilde{U}^{(l)} \} \}_{j \in \mathcal{N}})) \]

where \( \tilde{m}, \hat{\mu} \) and \( \hat{\phi} \) respectively apply the functions \( m, \phi \) and \( u \) simultaneously on each line of the local context \( \tilde{U} \). As the only non-zero line of \( \tilde{U} \) is \( \tilde{U}[i, :] \), \( 11^T \tilde{U}^{(l)} \) replicates the \( i \)-th line of \( \tilde{U}^{(l)} \) on all the other lines, so that they all share the same content \( x_i^{(l)} \). After the application of the message passing functions \( \tilde{m}, \hat{\phi} \) and \( \hat{\mu} \), all the lines of \( \tilde{U} \) therefore contain \( x_i^{(l+1)} \).

Finally, the function \( \text{diag} \) extracts the main diagonal of the tensor \( \tilde{U} \) along the two first axes. Let \( \delta_{i,j} \) be the function that is equal to 1 if \( i = j \) and 0, otherwise. We have:

\[ \text{diag}(\tilde{U})[i, j, :] = \tilde{U}[i, j, :] \delta_{i,j} \]

Note that this function can equivalently be written as an update function applied separately to each node:

\[ \text{diag}(\tilde{U})[j, :] = \tilde{U}[j, :] \delta_{i,j} \]

We now have \( \tilde{U}^{(l+1)}[i, :] = x_i^{(l+1)} \) and \( \tilde{U} \) equal to 0 on all the other entries, so that the induction hypothesis is verified at layer \( l + 1 \).

As any MPNN can be computed by an SMP, we conclude that SMPs are at least as powerful as MPNNs.

**SMP are strictly more powerful** To prove that SMPs are strictly more powerful than MPNNs, we use a similar argument to [23, 20].

**Lemma 6.** There is an SMP network which yields different outputs for the two graphs of Fig. 4 while any MPNN will view these graphs as isomorphic.

Figure 4: While MPNNs cannot distinguish between two regular graphs such as these ones, SMPs can.

**Proof.** The two graphs of Fig. 4 are regular, which implies that they cannot be distinguished by the Weisfeiler-Lehman test or by MPNNs without special node features [20]. On the contrary, consider an SMP \( f \) made of three layers computing \( \tilde{U}^{(l+1)} = \sum_{i \in \mathcal{N}_i} \tilde{U}^{(l)} \), followed by the trace of \( \tilde{U}^{(3)} \) as a a pooling function. As each layer can be written \( \tilde{U}^{(l+1)} = \tilde{A} \tilde{U}^{(l)} \) and \( \tilde{U}^{(0)} = I_n \), we have \( f(A) = tr(A^3) \). In particular \( f(A) = 2 \) for the graph on the left, while \( f(A) = 0 \) on the right.

**E  A more compact representation with graph coloring**

In SMP, the initial local context is a one-hot encoding of each node:

\[ \tilde{U}^{(0)} = \delta_i \in \mathbb{R}^\ell \]

When the graph diameter \( \Delta \) is large compared to the number of layers \( L \), the memory requirements of this one-hot encoding can be reduced by attributing the same identifiers to nodes that are far away from each other. In particular, no node should see twice the same identifier in its \( L \)-hop neighborhood.

To do so, we propose to build a graph \( G' \) where all \( 2L \)-hop neighbors of \( G \) are connected, and to perform a greedy coloring of \( G' \) (Algorithm 1). Although the number of colors \( \chi \) used by the greedy coloring might not be optimal, this procedure guarantees that identifiers do not conflict.
We will prove by induction that any Fast SMP layer can be approximated by two blocks of PPGN. It

Algorithm 1: Node coloring

**Input:** A graph $G = (V, E)$ with $n$ nodes, $L \in \mathbb{N}$ (number of layers).

**Output:** A binary matrix $U^0 \in \mathbb{R}^{n \times n}$, where $\gamma$ is the number of colors.

Create the graph $G' = (V, \{(i, j), d(i, j) \leq 2L\})$

c $\in \mathbb{R}^n \leftarrow$ greedy_coloring($G'$)

**return** one_hot_encoding($c$)

The one-hot encoding of the colors $U^0 \in \mathbb{R}^n$ is then used to initialize the local context of $v_i$. The only change in the SMP network is that in order to update the representation that node $i$ has of node $j$, we now update $U_i[c_j, :]$ instead of $U_i[j, :]$, where $c_j$ is the color associated to node $v_j$. Note however that the coloring is only useful if the graph has a diameter $\Delta > 2L$. This is usually the case in geometric graphs such as meshes, but often not in scale-free networks.

**F Proof of Proposition 2**

We will prove by induction that any Fast SMP layer can be approximated by two blocks of PPGN. It implies that the expressive power of Fast SMP is bounded by that of PPGN.

Recall that a block of PPGN is parameterized as:

$$T^{l+1} = m_4(m_3(T^{l}) \| m_1(T^{l}) \ast m_2(T^{l})),$$

where $m_k$ are MLPs acting over the third dimension of $T \in \mathbb{R}^{n \times n \times c}$: \forall $(i, j)$, $m_k(T)[i, j, :] = m_k(T[i, j, :])$. Symbol $\|$ denotes concatenation along the third axis and $\ast$ matrix multiplication performed in parallel on each channel: $(T \circ T')[i, j, c] = T[i, j, c] T'[i, j, c]$.

To simplify the presentation, we assume that:

- At each layer $l$, one of the channels of $T^{l}$ corresponds to the adjacency matrix $A$, another contains a matrix full of ones $\mathbf{1}_n \mathbf{1}_n^T$, and a third the identity matrix $I_n$, so that each PPGN layer has access at all times to these quantities. These matrices can be computed by the first PPGN layer and then kept throughout the computations using residual connections.

- The neural network can compute entry-wise multiplications $\odot$. This computation is not possible in the original model, but it can be approximated by a neural network.

- $U$ and $T$ have only one channel (so that we write them $U$ and $T$). This hypothesis is not necessary, but it will allow us to manipulate matrices instead of tensors.

**Initialization** Initially, we simply use the same input for PPGN as for SMP ($U^{(0)} = T^{(0)} = I_n$).

**Induction** Assume that at layer $l$ we have $U^{(l)} = T^{(l)}$. Consider a layer of Fast SMP:

$$U^{(l+1)} = \frac{1}{d_{avg}} \left( \sum_{v_j \in N_i} \hat{U}_j^{(l)} + \hat{U}_j^{(l)} W_4^{(l)} \odot \sum_{v_j \in N_i} \hat{U}_j^{(l)} W_5^{(l)} \right),$$

where

$$\hat{U}_j^{(l)} = U_j^{(l)} W_1^{(l)} + \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T U_j^{(l)} W_2^{(l)} + \mathbf{1}_n (c^{(l)})^T + \frac{1}{n} \mathbf{1}_n U_j^{(l)} W_3^{(l)}.$$

A first PPGN block can be used to compute $\hat{U}_j^{(l)}$ for each node. This block is parametrized by:

$$m_1(U^{(l)}) = \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T, \quad m_2(U^{(l)}) = U^{(l)},$$

$$m_3(U^{(l)}) = U^{(l)} W_1 + 1c^T + (I_n \odot U^{(l)}) W_3, \quad m_4(U, \tilde{U}) = \tilde{U} + \tilde{U} W_2 + I_n \odot (\tilde{U} W_3).$$

The output of this block exactly corresponds to $\hat{U}^{(l)}$. Then, a second PPGN block can be used to compute the rest of the Fast SMP layer. It should be parametrized as:

$$m_1([\hat{U}]^{(l)}) = A / \bar{d}, \quad m_2([\hat{U}]^{(l)}) = \hat{U}^{(l)},$$

$$m_3([\hat{U}]^{(l)}) = \hat{U}^{(l)}, \quad m_4(\hat{U}, \tilde{U}) = \tilde{U} + (\tilde{U} W_4) \odot (\tilde{U} W_5).$$
By plugging these expressions into the definition of a PPGN block, we obtain that the output of this block corresponds to $U^{(l+1)}$ as desired.

G Comparison of SMP and Provably powerful graph networks

Figure 5: Training curves of SMP and PPGN for different cycle lengths $k$. NLL stands for negative log-likelihood. Red dots indicate the epoch when SMP training was stopped. The training loss sometimes exhibits peaks of very high value which last one epoch – they were removed for readability. Provably powerful graph networks are much more difficult to train than SMP: their failure is not due to a poor generalization, but to the difficulty of optimizing them. We attribute this phenomenon to an inductive bias that is not suited to the task.