Should Graph Neural Networks Use Features, Edges, Or Both?

Lukas Faber, Yifan Lu, and Roger Wattenhofer

ETH Zurich, Switzerland

Abstract. Graph Neural Networks (GNNs) are the first choice for learning algorithms on graph data. GNNs promise to integrate (i) node features as well as (ii) edge information in an end-to-end learning algorithm. How does this promise work out practically? In this paper, we study to what extend GNNs are necessary to solve prominent graph classification problems. We find that for graph classification, a GNN is not more than the sum of its parts. We also find that, unlike features, predictions with an edge-only model do not always transfer to GNNs.

1 Introduction

Many complex real-world systems can be modeled as a graph, a set of nodes connected by edges. Graph Neural Networks (GNNs) have become a method of choice to apply learning in graphs. On a high level, each node comes with an initial set of features, which a GNN then translates into an embedding. For several rounds, nodes exchange and update their embeddings with their graph neighbors. The entire operations are differentiable, making GNNs essentially combine (i) the original *features* and (ii) the *edges* of the graph into an end-to-end learning algorithm. In this paper we study whether this intuition about GNNs is true. Do the prominent GNN problems use both (i) features *and* (ii) edges? To what extent can a dataset be solved with only features *or* edges? How well do GNNs to exploit the combination of features and edges, i.e., is the combination more than the sum of the parts (as in Figure 1)?

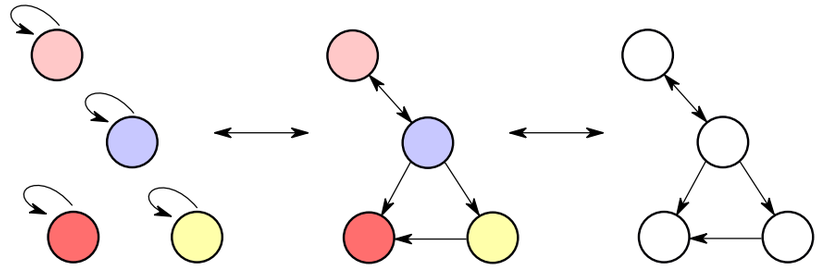


Fig. 1: A GNN (center) is the composition of a feature-only model (left) and an edge-only model (right).

Work inspired by the paper:
"Pitfalls of GNN evaluation" from TUM

The contributions of this paper can be summarized as follows:

- We present two measures, FandE (Features and Edges) and ForE (Features or Edges) to quantify for a dataset to what extent we can use edges and features to solve its predictions. A high ForE score means that GNNs are not necessary for solving a dataset.
- In experiments on popular datasets, we find that several eminent datasets are largely solved by *only* features or edges and thus do not need GNNs. We believe that these datasets should be supplemented with datasets with a lower ForE.
- We further present GaP (GNNs and its Parts). GaP measures to what extent a GNN can solve predictions neither features nor edges can solve and to what extent GNNs can also solve what either of those models could solve.
- In experiments on existing architectures and datasets, we show that current GNN models are better in node classification than graph classification.

2 Related Work

2.1 GNN Architectures

One of the pioneering works is the GNN model by Scarselli et al. [20]. There, nodes have an embedding that is propagated and updated with their neighbors until convergence. The final embeddings are used for prediction, receive an error signal, and update. Since then, many further GNN models were proposed that generally follow the message passing paradigm [7]. Similar to Scarselli et al., nodes in this framework have embeddings, they create messages based on these embeddings, send those messages to their neighbors, and update their embeddings based on received messages. There are many different instantiations of this message passing framework [25], for example some based on spectral graph theory [3,12], (self-) attention [13,23], convolution operations [17,26] or residual connections [27].

2.2 Datasets for GNN Evaluation

Currently, many GNN architectures are evaluated on the same datasets. However, current research investigates how appropriate these datasets are for benchmarking GNNs. Zou et al. [31] show that the prominent Cora and Citeseer datasets leak label information in their features, thus allowing several shortcuts in predicting node labels. Huang et al. [10] highlight another property of commonly used node classification datasets: homophily. Exploiting this property with an enhanced label propagation algorithm, they can achieve superior performance over GNNs. Zhu et al. [30] examine the interplay between homophily in datasets and GNN performance. They find many current datasets to be biased towards homophily. In this paper, we propose a novel measure, ForE, to quantify the difficulty of a dataset (if we can solve the dataset without GNNs)

What does "leak label information" mean? just look at citation

ForE: difficulty of a dataset

without GNNs just means that either only edge information or node information without propagation is enough to solve the task

and find that several prominent datasets are indeed easy to solve using only features *or* edges. We argue future GNN evaluation should rely on more challenging datasets. There are several data collections available [4, 9, 15, 16, 22], from which we can further assemble datasets and evaluate those datasets with ForE.

2.3 Limitations of current GNNs

Despite the numerous new GNN architectures in recent years, the current theoretical and practical shortcomings in GNNs will require better architectures. From a theoretical perspective, GNNs cannot fully differentiate between different structures [6, 26], thus they do not understand the full capabilities of graphs. From a practical perspective, most current GNN architectures are limited to shallow models or suffer from the oversmoothing effect [2, 14, 18, 29]. Thus, models are limited to few layers. This restricts every node to extract local information only. Furthermore, existing empirical differences between GNN architectures are smaller than thought [21]. To foster further evaluation of GNNs, we contribute a new dimension on how to go forward evaluating GNNs parallel to benchmark high-scores. A GNN should encompass the predictions of its parts: features and edges. This measure shows already one potential angle of improvement since current GNN architectures cannot always preserve the predictions of an edge-only model.

3 Background

3.1 Examined Problems.

In this paper, we consider the two prominent tasks in graph machine learning: Node classification and graph classification. In node classification, we usually have a single graph that is partially labeled. The aim is to train a model to classify all unlabeled nodes. In graph classification, we have a collection of training graphs where each graph has a label. The aim is to train a model to learn to classify further unseen graphs. Here, we unify both tasks under the framework of having to make predictions. Thus, a prediction can be assigned a label to a node or a graph and thus a prediction can be correct or wrong. Generally, we are interested to measure how many correct predictions a certain model does.

3.2 Perspective on GNNs.

Almost all GNN architectures [3, 8, 12, 23, 25–27] follow the message passing framework [7]. Every node starts with an embedding given by its initial features. One round of message passing then consists of nodes creating a message based on this embedding, sending this message to their neighbors, collect and aggregate all received messages, and finally updating their embedding on the received information. Usually, a GNN performs some number k rounds of message passing. Thus, the node's embedding in a GNN does reflect its features and

Their main point is that more difficult datasets should be used to evaluate GNNs that cannot be "solved" with, for instance, Label propagation

the information of its $k-$hop neighborhood. In the case of a graph classification problem, we read out a graph-level representation by summing up node embeddings. Compared to models that can only leverage either features or edges (the neighborhood information), a GNN has a superset of information. A GNN is a composition of both approaches (as in Figure 1). In this paper, we will investigate how much simpler models can sufficiently tackle various datasets and how much a GNN composition does improve over its parts.

4 ForE and GaP

In this section, we define the measures of ForE and GaP. Both measures are built upon investigating the predictive power of two baseline models: a feature-only model and an edge-only model, which we will define in Section 4.1. We measure the predictive power of these models through the *set of solvable nodes (solvable set)*. We define this set in Section 4.2. Next, we introduce ForE in Section 4.3. Here, we measure the ratio of nodes that are not in the union of the solvable sets of a feature-only and an edge-only model—that is for which we need the composed GNN model to hope for correct predictions. Last, we define GaP in Section 4.4: The solvable set of a GNN should contain the solvable set of both a feature-only and an edge-only model, plus additional nodes. Such GNNs are indeed more than the sum of its parts.

4.1 Feature-Only and Edge-Only Models

A GNN combines a feature-only model and an edge-only model into a single model. We will illustrate this concept with the example of the GCN model [12]. Here, node embeddings for layer $l+1$ are derived according to:

$$H^{(l+1)} = \sigma(D^{\frac{1}{2}}AD^{\frac{1}{2}}H^{(l)}W^{(l)}) \tag{1}$$

For the **Feature-Only** model, we stack the node features into a $node \times feature$ input matrix and feed this matrix through a multilayer feedforward network. Thus, every set of node features gets exposed to a set of weight matrices and nonlinear activations. This is equivalent to the multiplication with $W^{(l)}$ and final activation with a nonlinearity σ in the GCN model (see Equation (1)). As alternative, less architecturally aligned choices, we could employ any "classical" machine learning algorithm to predict labels, given an $sample \times feature$ input matrix. One particularly interesting alternative algorithm could be a tree-based model which allows for higher interpretability and might indicate how a model can predict certain nodes.

For the **Edge-Only** model, we use the actual GNN propagation — except we replace the initial node features with an all-ones vector. That is, in Equation (1), we replace $H^{(0)}$ with a same shaped all-ones matrix. As other edge-only models, we considered extracting features manually and providing every node these features (such as its degree, pagerank, centrality measure,...). However,

Use node-wise MLP as node/feature-only model

← So the Edge-Only model only has the graph topology

we believe allowing the model to extract relevant features itself to be the better and more flexible approach. As another alternative, we see label propagation algorithms, as were used by Shchur et al. [21]. However, these approaches require label information during inference time, which we cannot provide for the inductive graph classification problem.

4.2 Solvable Sets

In this section, we define the solvable set of predictions for a model. One possible approach would be instantiating a model several times and averaging the instance accuracies. We see this approach having two drawbacks: We do not capture the consistency in which model instances predict a certain prediction correctly and second, more importantly, the score will depend on the number of classes. In the extreme case of binary classification, even a random model will predict 50% correctly. Therefore, we present another model that is independent of the number of classes and identifies only consistently correct predictions.

Across many instantiations of a model (through multiple independent runs), we investigate if the model is *significantly more often* correct about a prediction than what we can explain through random guessing. Therefore, per prediction, we test the null hypothesis that the different runs can only predict correctly through chance. These runs are independently initialized, therefore, we assume that the events of correct random guesses are also independent of each other. Thus we expect the random guesses to follow a Bernoulli Distribution with a success probability $p = \frac{1}{c}$ with c being the number of possible classes. If we can reject the null hypothesis for a prediction, we can conclude that the data contains information that allows us to systematically predict correctly. These are the predictions we consider solved; the solvable set of a model is the set of all solved predictions. Formally, for a universe of predictions of a dataset P, the solvable set of a model M is defined as $S(M) = \{p \in P | M \text{ solves } p\}$. Note that this measure does not directly relate to a particular instance that does the correct prediction, but having one instance (or some ensembled instances) will allow us to get the right prediction.

4.3 ForE

Equipped with computing the solvable sets for feature-only and edge-only models, we quantify datasets on the question: Does this dataset even need a GNN to solve? We would consider a GNN necessary for a prediction when neither the simpler feature-only or edge-only model suffices. We can quantify this as $\text{ForE} = \frac{|S(Features) \times S(Edges)|}{|P|}$. Ideally, we evaluate GNNs on challenging datasets where all predictions would require joint feature and edge information. A more realistic stance is that we do not want all predictions solved by looking only at the features or edges. Naturally, we can address these predictions with a GNN as well, but such a dataset does not allow us to measure how much new predictive power a new GNN architecture offers. This is because the GNN just has to learn

This should be all the labels in our dataset that we can consistently correctly predict over multiple training runs.
Why not majority classifier instead of uniformly random as the null hypothesis? they have not thought of this's
Train multiple seeds and see what labels we significantly more often predict correctly than random guessing.
Null hypothesis: We are just randomly guessing
if we reject the null hypothesis, then that label is in the solvable set.
P: all the labels
M: model that is trained multiple times
S(M): Labels that M gets correct ("solvable labels") often
typo: they actually mean union
that would mean $\text{ForE} = \frac{0}{|P|} = 0$
#of labels that can be solved by both simple models
$\text{ForE} = \frac{|S(Features) \cup S(Edges)|}{|P|}$
#labels
If the simple models can solve all labels easily, we have ForE = 1
⇒ We want a low ForE for our datasets

to use either the features only or the nodes. Therefore, we would like datasets to have a low ForE value.

4.4 GaP

As a second application for solvable sets, we now continue to answer: Are current GNNs more than the sum of their parts? A GNN has access to all the information of its parts, plus it can additionally exploit having both features at the same time. Therefore, what we would like to see are three effects: The solvable set of the GNN is a superset of the solvable set of both the feature-only and the structure-only model. We measure this property by computing the ratio $\frac{|S(\text{GNN}) \cap S(\text{Features})|}{|S(\text{Features})|}$ and $\frac{|S(\text{GNN}) \cap S(\text{Edges})|}{|S(\text{Edges})|}$, respectively. An effective GNN will achieve values close to 1. Moreover, an effective GNN should exploit having the joint information of features and edges to make predictions, which neither individual model is capable of. We measure this extent as $\frac{|S(\text{GNN}) \cap \text{U}|}{|\text{U}|}$ where U is the set of "unsolved" nodes $U = P \setminus (S(\text{Features}) \cup S(\text{Edges}))$. In an ideal world, a GNN would be able to solve all remaining predictions thus yielding a perfect score of 1; however, we expect real values to turn out lower due to data errors, labeling noise, and similar effects.

GaP should answer if
$S(GNN) > |S(Features) \cap S(Edges)|$

U: Labels that cannot be solved by either of the simple models

$GaP = \frac{|S(GNN) \cap U|}{|U|}$ ← how many GNN can solve which simple models could not solve

↑ #Labels that the simple models cannot solve

5 Experiments

We investigate prominent GNN architectures and GNN benchmarking datasets using ForE and GaP. We choose to run experiments with four archetypes of established GNN models: Graph Convolutional Networks (GCN) [12], GraphSage (GS; pooling and mean variants) [8], Graph Attention Networks (GST) [23], and Graph Isomorphism Networks (GIN; max, mean, and sum variants) [26]. For datasets, we choose from a variety of dataset collections, covering a variety of domains. We use transductive node classification datasets stemming from citation networks (Cora, Citeseer, Pubmed, OGBN-Arxiv), co-purchasing graphs (AMZN-Photo, AMZN-Comp) from Amazon [15], and coauthorship networks based on the Microsoft Academic Graph [22] (MAG-Physics, MAG-CS). For choosing the subsets of the Microsoft Academic Graph and the amazon co-purchasing data, we follow the choice of Shchur et al [21]. On the other hand, we experiment with several inductive graph classification tasks from the dataset collection of Morris et al. [16]. In Mutag, the task is to predict the chemical properties of molecules. The datasets Proteins and Enzymes come from the biology domain and classify if a protein is an enzyme or which kind of enzyme, respectively. The dataset Reddit-B is about classifying Reddit threads where nodes are users and edges for answering users whether this thread is a discussion or a Q&A session. The last dataset IMDB-M is a dataset to detect the genre of movies based on a network of actor collaborations. Most datasets come with a suggested split for the predictions into the training, validation, and test set, which we keep. In case there is no such split, we create one fixed split.

None of the models use edge information!!

The edge model only uses the graph topology, no features at all.

5.1 Hyperparameter settings

We use the implementation provided by the DGL library [24] for GNN implementation, keeping the hyperparameters to their default values. We set the number of layers of the GNNs to 3 and the embedding width to be twice the number of input or output values — whichever is larger. Several datasets have a massive number of features (for example), which is why we upper bound the embedding size to 128. We train the GNNs for up to 10.000 epochs with early stopping on the validation metrics with patience of 25. In practice, we find that training generally needs much fewer epochs, and models converge after several hundred epochs. Models are trained with the Adam optimizer [11] and its default parameters in the PyTorch library [19]. To ensure structural similarity with the GNNs, we employ a 3 layer feedforward network, which we train in the same fashion. For the edge-only model, we try all GNN propagation and pick the best one per dataset. We run each dataset model configuration 100 times with different random seeds and do the statistical test with a 99.9% confidence level ($p = 0.001$).

Why not use conventional settings for the respective datasets? Maybe the poor parameter choices cause the low gap in many cases

5.2 ForE Results

Table 1 shows results, for solvable sets of feature-only, edge-only models, their expected FandE (assuming independence), the actual FandE, ForE, and the solvable set of the best-performing GNN. All node classification datasets behave very similarly: 1) Using only features, we can solve a large portion of the dataset; 2) the edge-only model is a useful and mostly independent additional source of information; 3) GNNs perform better than either. The most important observation is, however, that ForE is rather high for most datasets, especially for the MAG based datasets.

For graph classification datasets, we observe that the performance for features and edges is similar. Furthermore, the solvable sets of features and edges are not independent but correlate. This suggests that there are "easy" graphs that we can predict either way. For almost all datasets, no GNN architecture offers an of-the-shelf-advantage over features or nodes.

5.3 GaP

We now further investigate the performance of GNNs compared to their parts. First, we take a look if GNNs can solve those predictions its parts also solve. Figure 2 shows results for these experiments. In Figure 2a we can see the ratio of solved predictions the GNN preserves from the feature-only model; Figure 2b shows the prediction from the edge-only model. We can observe that GNNs are consistently good at preserving feature predictions. For edge predictions the picture is less clear, for some datasets, the GNN can only preserve around two thirds. This gap allows for improving scores, for example through ensembling GNNs and feature-only models.

Dataset	Features	Edges	$\mathbb{E}$(FandE)	FandE	ForE	GNN
Cora	0.586	0.346	0.203	0.192	0.74	0.828
Citeseer	0.544	0.412	0.224	0.235	0.721	0.699
Pubmed	0.693	0.407	0.282	0.246	0.854	0.779
AMZN-Photo	0.777	0.286	0.222	0.172	0.891	0.909
AMZN-Comp	0.652	0.391	0.255	0.235	0.808	0.809
MAG-Physics	0.915	0.507	0.464	0.475	0.947	0.949
MAG-CS	0.924	0.136	0.126	0.129	0.932	0.933
OGBN-Arxiv	0.658	0.411	0.271	0.281	0.788	0.726
Mutag	0.45	0.55	0.248	0.45	0.55	0.55
Enzymes	0.4	0.333	0.133	0.2	0.533	0.65
Proteins	0.607	0.643	0.39	0.607	0.643	0.616
IMDB-M	0.26	0.293	0.076	0.24	0.313	0.287
Reddit-B	0.76	0.775	0.589	0.76	0.775	0.77

Node prediction

Graph prediction

Table 1: We analyzed 8 node prediction and 5 graph prediction datasets. We report their prediction score based on Features only and Edges only in Columns 2 and 3. $\mathbb{E}$(FandE) shows the expected ratio that Features and Edges are correct, assuming independence. FandE reports the actual overlap between Features and Edges. ForE reports the ratio of predictions that at least one of Features and Edges solve. GNN shows the correct predictions for the best-performing GNN on this dataset. Let us look at the example dataset MAG-CS. From columns 2 and 3 we learn that using just features or edges we can solve 92.4% or 13.6% of the predictions of this dataset, respectively. Columns 4 and 5 show that the expectation of FandE is close to the actual value, suggesting that features and edges are independent sources of information. The ForE shows that 93.2% of all predictions can be solved with features or edges and do not need a GNN. Last, the best-performing GNN model solves 93.3% of all nodes.

Last, we wonder if GNNs are more than the combination of their parts. We look at the ratio of the unsolved nodes that a GNN can solve in Figure 3. In all node classification datasets apart from the dataset OGBN-Arxiv, GNNs solve a large fraction of nodes neither features nor edges can do. On the other hand, we see there is a gap in expressive power for graph classification problems. GNNs do hardly solve further predictions. Across all experiments, all investigated GNN architectures perform virtually the same, except for few outliers from GAT. In general, we establish this trend in Figure 4. Every cell shows the Jaccard similarity of solvable sets across all datasets between two GNN architectures. We can see that every pair of architectures achieve similarities close to 1. This suggests that all GNN architectures solve more or less the same predictions.

$$\text{Features is } \frac{|S(\text{Features})|}{|P|}$$

$$\text{ForE} = \frac{|S(\text{Feat}) \cup S(\text{Edges})|}{|P|}$$

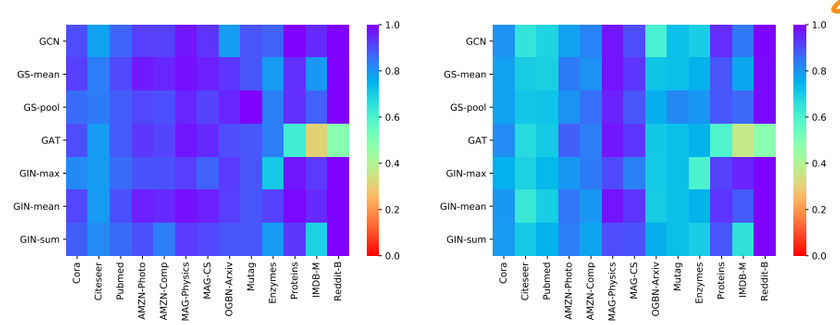
$$\text{GNN is } \frac{|S(\text{GNN})|}{|P|}$$

$$\text{FandE} = \text{ForE} = \frac{|S(\text{Feat}) \cap S(\text{Edges})|}{|P|}$$

this is $\frac{|S(GNN) \cup S(Features)|}{|S(Features)|}$

This is in line with the finding of Shchur et al [21] that find similar performance across architectures.

a lot of labels that are solved by the edge only model are not solved by the GNN



(a) (b)

Fig. 2: How much can a GNN replace its parts? Per cell, we show the ratio of predictions and feature-only model (a) or an edge-only model (b) can solve that a GNN can also solve (higher values are better). For example, consider the entry for GCN and Citeseer in Figure 2b (first row, second column). The score of 64.6% indicates that only around 2 out of 3 predictions of the edge-only model solves are also solved by the GNN. This motivates new GNN architectures that preserve more predictions or cleverly ensemble GNNs with its edge-only parts.

6 Conclusion

GNNs as a machine learning model provide us with an algorithm to jointly use the node features and edges. We present ForE to measure if datasets even require this capability and to what extent they can only be solved through one input. We presented GaP, to measure if GNNs can preserve the predictions of its parts and if GNNs are more than their sum. From the experiments, we draw the following conclusions:

– We should rethink which datasets to use for GNN evaluation. From Zou et al. [31] and Huang et al. [10], we know that Cora and Citeseer are not ideal datasets. Additionally, we now know that also many other node classification datasets are “easy” due to having a high ForE score. Especially the MAG-based datasets are virtually solved through features alone. Such datasets let us hardly measure the new expressive power of GNNs but rather a GNN’s ability to harness these features.
– We should be able to improve current GNN performance by ensembling GNN models with edge-only models. Figure 2b shows that GNNs do not preserve

GaP = $\frac{|S(GNN) \cap U|}{|U|}$ (U: unsolved by simple model(s))

Jaccard similarity = $\frac{\text{intersection}}{\text{union}}$ 

so it is 1 if the two sets are the same

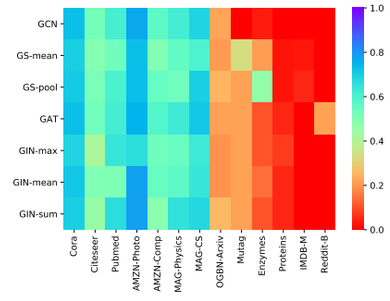


Fig. 3: To what extent is a GNN more than the sum of its parts? Per cell, we show the ratio of predictions that neither features nor edges can solve, but a GNN can (higher values are better). For example, the value for GCN in Cora is 70.4%. This means that a GCN can solve this percentage of predictions that are not in ForE (see Table!1). Thus, the GCN contributes predictions we could not do without it.

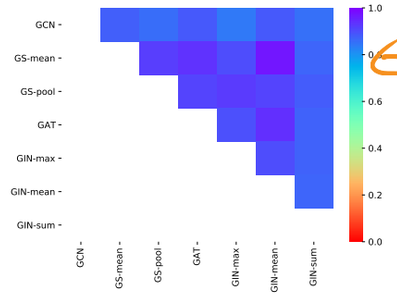


Fig. 4: To what extent do solvable sets of different GNN architectures overlap? Per cell, we show the Jaccard similarity between GNN solvable sets over all datasets. For example, the Jaccard Similarity between GS-mean and GIN-mean is 97.1%. This shows that across all datasets, the two architectures can solve virtually the same nodes. Despite their differences in Architecture, their predictive power seems to be equal.

← Jaccard similarity between solvable sets of the networks ⇒ almost all solve the same labels (averaged across all datasets)

all correct predictions (unlike feature predictions). This also motivates further research into GNN architectures that preserve edge predictions better.

– Currently, GNNs are better at node classification than graph classification. We come to this conclusion because, on the one hand, GNNs outperform both feature-only and edge-only in node classification datasets (see Table 1). On the other hand, GNNs generally solve more predictions than their parts for node classification (see Figure 3). This suggests that the current approach of node-level propagation and doing a graph-level readout through summation is not as effective. This motivates further research on dedicated graph classification architectures. Two example ideas are master nodes that gather global information [7] or graph pooling to aggregate node embeddings [1, 5, 13, 28].
– All previous observations hold almost independent of the chosen GNN architecture (the rows in Figures 2a, 2b, and 3 are similar, while there are large differences per column). Furthermore, all GNN architectures yield similar observable sets (see Figure 4). Going forward, we consider it promising to again look beyond message passing to potentially diversify the solvable sets.

Isn't this pure speculation and the observations are just completely dependant on the type of data?

References

1. Cangea, C., Veličković, P., Jovanović, N., Kipf, T., Liò, P.: Towards sparse hierarchical graph classifiers. arXiv:1811.01287 (2018)

2. Chen, D., Lin, Y., Li, W., Li, P., Zhou, J., Sun, X.: Measuring and relieving the over-smoothing problem for graph neural networks from the topological view. In: Conference on Artificial Intelligence (AAAI), New York, USA (Feb 2020)
3. Defferrard, M., Bresson, X., Vandergheynst, P.: Convolutional neural networks on graphs with fast localized spectral filtering. In: Advances in neural information processing systems (2016)
4. Dwivedi, V.P., Joshi, C.K., Laurent, T., Bengio, Y., Bresson, X.: Benchmarking graph neural networks. arXiv:2003.00982 (2020)
5. Gao, H., Ji, S.: Graph u-nets. arXiv:1905.05178 (2019)
6. Garg, V., Jegelka, S., Jaakkola, T.: Generalization and representational limits of graph neural networks. In: International Conference on Machine Learning (ICML), virtual (Jul 2020)
7. Gilmer, J., Schoenholz, S.S., Riley, P.F., Vinyals, O., Dahl, G.E.: Neural message passing for quantum chemistry. In: International Conference on Machine Learning (ICML), Sydney, Australia (Aug 2017)
8. Hamilton, W., Ying, Z., Leskovec, J.: Inductive representation learning on large graphs. In: Advances in neural information processing systems (2017)
9. Hu, W., Fey, M., Zitnik, M., Dong, Y., Ren, H., Liu, B., Catasta, M., Leskovec, J.: Open graph benchmark: Datasets for machine learning on graphs. arXiv:2005.00687 (2020)
10. Huang, Q., He, H., Singh, A., Lim, S.N., Benson, A.R.: Combining label propagation and simple models out-performs graph neural networks. arXiv:2010.13993 (2020)
11. Kingma, D.P., Ba, J.: Adam: A method for stochastic optimization. In: Bengio, Y., LeCun, Y. (eds.) International Conference on Learning Representations ICLR 2015, San Diego,USA (May 2015)
12. Kipf, T.N., Welling, M.: Semi-supervised classification with graph convolutional networks. In: International Conference on Learning Representations ICLR, Toulon, France (Apr 2017)
13. Lee, J., Lee, I., Kang, J.: Self-attention graph pooling. In: International Conference on Machine Learning (ICML), Long Beach, USA (Jun 2019)
14. Li, Q., Han, Z., Wu, X.M.: Deeper insights into graph convolutional networks for semi-supervised learning. In: Conference on Artificial Intelligence (AAAI), New York, USA (Feb 2018)
15. McAuley, J., Targett, C., Shi, Q., van den Hengel, A.: Image-based recommendations on styles and substitutes. In: ACM SIGIR Conference on Research and Development in Information Retrieval (SIGIR), Santiago, Chile (Aug 2015)
16. Morris, C., Kriege, N.M., Bause, F., Kersting, K., Mutzel, P., Neumann, M.: Tudataset: A collection of benchmark datasets for learning with graphs. arXiv:2007.08663 (2020)
17. Niepert, M., Ahmed, M., Kutzkov, K.: Learning convolutional neural networks for graphs. In: International Conference on Machine Learning (ICML), New York, USA (Jun 2016)
18. Oono, K., Suzuki, T.: Graph neural networks exponentially lose expressive power for node classification. In: 8th International Conference on Learning Representations (ICLR), Addis Ababa, Ethiopia (Apr 2020)
19. Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein, N., Antiga, L., Desmaison, A., Kopf, A., Yang, E., DeVito, Z., Raison, M., Tejani, A., Chilamkurthy, S., Steiner, B., Fang, L., Bai, J., Chintala, S.: Pytorch: An imperative style, high-performance deep learning library. In: Advances in Neural Information Processing Systems (2019)

20. Scarselli, F., Gori, M., Tsoi, A.C., Hagenbuchner, M., Monfardini, G.: The graph neural network model. IEEE Transactions on Neural Networks (2008)
21. Shchur, O., Mumme, M., Bojchevski, A., Günnemann, S.: Pitfalls of graph neural network evaluation. arXiv:1811.05868 (2018)
22. Sinha, A., Shen, Z., Song, Y., Ma, H., Eide, D., Wang, K.: An overview of microsoft academic service (mas) and applications. In: International Conference on World Wide Web (WWW), Florence, Italy (May 2015)
23. Velickovic, P., Cucurull, G., Casanova, A., Romero, A., Liò, P., Bengio, Y.: Graph attention networks. In: International Conference on Learning Representations (ICLR), Vancouver, BC, Canada (May 2018)
24. Wang, M., Zheng, D., Ye, Z., Gan, Q., Li, M., Song, X., Zhou, J., Ma, C., Yu, L., Gai, Y., Xiao, T., He, T., Karypis, G., Li, J., Zhang, Z.: Deep graph library: A graph-centric, highly-performant package for graph neural networks. arXiv:1909.01315 (2019)
25. Wu, Z., Pan, S., Chen, F., Long, G., Zhang, C., Philip, S.Y.: A comprehensive survey on graph neural networks. IEEE Transactions on Neural Networks and Learning Systems (2020)
26. Xu, K., Hu, W., Leskovec, J., Jegelka, S.: How powerful are graph neural networks? In: International Conference on Learning Representations, ICLR 2019, New Orleans, USA (May 2019)
27. Xu, K., Li, C., Tian, Y., Sonobe, T., Kawarabayashi, K.i., Jegelka, S.: Representation learning on graphs with jumping knowledge networks. In: International Conference on Machine Learning (ICML), Stockholm, Sweden (Jul 2018)
28. Ying, Z., You, J., Morris, C., Ren, X., Hamilton, W., Leskovec, J.: Hierarchical graph representation learning with differentiable pooling. In: Advances in neural information processing systems (2018)
29. Zhao, L., Akoglu, L.: Pairnorm: Tackling oversmoothing in gnns. In: International Conference on Learning Representations (ICLR) 2020, Addis Ababa, Ethiopia (Apr 2020)
30. Zhu, J., Yan, Y., Zhao, L., Heimann, M., Akoglu, L., Koutra, D.: Beyond homophily in graph neural networks: Current limitations and effective designs. Advances in Neural Information Processing Systems (2020)
31. Zou, X., Jia, Q., Zhang, J., Zhou, C., Yang, H., Tang, J.: Dimensional reweighting graph convolutional networks. arXiv:1907.02237 (2019)