Toward the Analysis of Graph Neural Networks

Thanh-Dat Nguyen* thanhdatn@student.unimelb.edu.au University of Melbourne Melbourne, Victoria, Australia Thanh Le-Cong* thanh.ld164834@sis.hust.edu.vn Hanoi University of Science and Technology Hanoi, Vietnam ThanhVu H. Nguyen tvn@gmu.edu George Mason University Fairfax, Virginia, Vietnam

Xuan-Bach D. Le bach.le@unimelb.edu.au University of Melbourne Melbourne, Victoria, Australia Quyet-Thang Huynh thanghq@soict.hust.edu.vn Hanoi University of Science and Technology Hanoi, Vietnam

ABSTRACT

Graph Neural Networks (GNNs) have recently emerged as a robust framework for graph-structured data. They have been applied to many problems such as knowledge graph analysis, social networks recommendation, and even Covid19 detection and vaccine developments. However, unlike other deep neural networks such as Feed Forward Neural Networks (FFNNs), few analyses such as verification and property inferences exist, potentially due to dynamic behaviors of GNNs, which can take arbitrary graphs as input, whereas FFNNs which only take fixed size numerical vectors as inputs.

This paper proposes an approach to analyze GNNs by converting them into FFNNs and reusing existing FFNNs analyses. We discuss various designs to ensure the scalability and accuracy of the conversions. We illustrate our method on a study case of node classification. We believe that our approach opens new research directions for understanding and analyzing GNNs.

KEYWORDS

Property Inference, Formal Explanations, Graph Neural Networks

ACM Reference Format:

Thanh-Dat Nguyen, Thanh Le-Cong, ThanhVu H. Nguyen, Xuan-Bach D. Le, and Quyet-Thang Huynh. 2022. Toward the Analysis of Graph Neural Networks. In *Proceedings of The 44th International Conference on Software Engineering (ICSE 2022).* ACM, New York, NY, USA, 5 pages. https://doi.org/10.1145/nnnnnnnnn

1 INTRODUCTION

Deep Neural Networks (DNNs) have emerged as one of the most effective and modern approaches in solving problems, from common ones such as movies recommendations, image recognition

ICSE 2022, May 21-29, 2022, Pittsburgh, PA, USA

© 2022 Association for Computing Machinery.

ACM ISBN 978-x-xxxx-x/YY/MM...\$15.00

https://doi.org/10.1145/nnnnnnnnnnnn

to important ones such as collision control and "fake" news and information detection. Just like software, these DNN models can be misused and attacked (e.g., small perturbations to the inputs can result in misclassifying results). Thus, over the last decade, researchers have developed many powerful techniques to analyze DNNs, e.g., verifying that for certain inputs, a DNN will result in a certain output or have a desirable property, and more recently, inferring properties or facts to help explain behaviors of a DNN, which is typically treated as blackbox.

Despite the proliferation of DNNs analyses, most effective ones focus only on certain types of DNNS, such as Feedforward Neural Network (FFNNs), in which the inputs are presented as fixed-size vectors of numbers and a fixed structure network. One of the more complicated DNNs that has recently been used in practice is Graph Neural Networks (GNNS), which take inputs as *graphs* of various sizes (even each of the nodes in the graph is attached with information encoded as a vector of numbers) and have a dynamic network that depends on the structure and information from the input graphs. GNNs have been applied to solve many practical problems, e.g., knowledge graphs analysis [12], recommendation system for social networks [16], chemical and protein classification [4, 10], reasoning the structure of graphics and images [13], and even advanced COVID19 detection [11, 19] and vaccine development [2, 6, 17].

Just as with standard DNNs, complex GNNs are often used as blackbox and can be vulnerable to adversary attacks, all of which lead to concerns about safety, fairness, and privacy of GNNs [3, 14, 18], e.g., a new Covid vaccine developed by unknown and attackedprone ML technique can only further increase doubts and hesitancy from the public. However, unlike popular FFNNs, in which there are many effective formal analyses, to the best of our knowledge, few exist for GNNs, potentially due to the vast differences between the two types of networks.

In this paper, we propose an approach to analyze GNNs, both in verification and property inference, by converting GNNs to FFNNs and reusing developed techniques for FFNNs. While analyses explicitly designed for GNNs can be more efficient, they can be difficult and time-consuming to develop due to the differences between two types of networks. Thus, we believe our approach of leveraging existing efficient techniques and tools can be achieved quicker and also as effectively, as we can rely on existing powerful FFNN tools. This kind of approach is similar to many techniques in software

^{*}Both authors contributed equally to this research.

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than ACM must be honored. Abstracting with credit is permitted. To copy otherwise, or republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from permissions@acm.org.

ICSE 2022, May 21-29, 2022, Pittsburgh, PA, USA

Thanh-Dat Nguyen, Thanh Le-Cong, ThanhVu H. Nguyen, Xuan-Bach D. Le, and Quyet-Thang Huynh

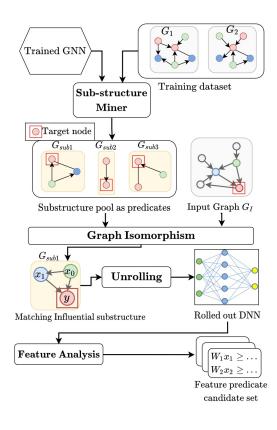


Figure 1: Overview

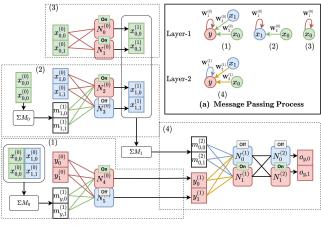
engineering that encode the analysis task as a logical formula that can be efficiently analyzed by existing constraint solving techniques and tools (e.g., SAT and SMT solvers).

Fig. 1 gives an overview of our idea. The main challenge in analyzing GNNs and converting them to FFNNs is that the input graphs of a GNN can have various topological structures and the GNN has a dynamic structure depending on its input graphs. To solve this challenge, we mine influential sub-structures of input graphs to summarize the structural input space of a GNN. Then for each sub-structure, which represents a class of input graphs, we "unroll" the structure to create an equivalent FFNN for each node update operation of GNN, and then combine these FFNNs into a final FFNN representing the original GNN computation of the substructure. While influential substructure should contribute significantly toward GNN prediction, additional nodes that are noninfluential can still affect the final computation result of the GNN. To deal with this, we find conditions on which the rolled out FFNN on the substructure and the original GNN is equivalent to ensure our results.

Finally, given the equivalent condition, we can now extend the existing DNN analyses to the rolled out FFNN of each substructure and obtain results for the original GNN.

2 TECHNICAL APPROACH

Existing verification techniques for DNNs attempt to check that the DNN satisfies a user-supplied property (e.g., a certain range over



(b) Feed forward Neural Network

Figure 2: GNN message passing and unrolling

inputs results in a certain output). In contrast, property inference attempts to automatically infer such properties from the DNN. In both cases, the property to be verified or inferred has the form pre \implies post, where pre is a condition over the inputs and post is certain requirement on the outputs. Typically, we are interested in verifying or inferring the pre for some specific post, e.g., we want to find input conditions that make the DNN classifies an image as a "dog".

For this work, we will consider GNN models for the standard problem of graph node classification, which takes as input a graph *G* and gives a classification *c* for each node $v \in G$. For such GNNs, the pre are *input properties*, which are logical *predicates* capturing common structure and features¹ of the input graphs that lead to a certain classification of the target node. Below we use a concrete example given in Fig. 2 to describe the steps of our approach, whose overview is given in Fig. 1.

2.1 Substructure Mining

Unlike an FFNN, a GNN does not have a fixed structure: it can take arbitrary graphs and the behaviors of GNN itself also change depending on the structure of the inputs (e.g., the influence of a node depends on its neighbors). Thus, a direct, naïve way of converting a GNN to an FFNN does not scale as it would result in a different FFNN for each different input graph and the FFNN can also be very large if the input graph is large.

To solve this challenge, we will create FFNNs that support *classes* of input graphs. We leverage existing works in network graphs and GNNs to mine common and influential *substructures* from sample input graphs. These substructures are compact and summarize important behaviors of a GNN[9, 15], and existing works such as GNNExplainer and PGExplainer [9, 15] can extract substructures that are important to each GNN prediction (e.g., sets of edges, nodes,

¹Node features are attributes of nodes, e.g., if we take a node "professor" in academic graph, its attributes may be "name", "citations", "affiliation", and encoded as a numerical vector such as {0.1, 0.3, 0.4, 0.5}.

ICSE 2022, May 21-29, 2022, Pittsburgh, PA, USA

and features that are important to the output of target node's prediction). These substructures are crucial for the generation and analysis of FFNNs in subsequent tasks. For example, comparing to individual graphs these influential substructures are compact, which are crucial to achieving FFNNs with manageable sizes.

Fig. 1 illustrates how we mine influential substructures (*sub-structure miner*). For a trained GNN model, we take in a set of input graphs that have the desired classification and use an existing tool such as GNN explainer to extract subgraphs that are common from the input graphs and influential to the classification result of the target node. In Figure 1, from the two input graphs G_1 and G_2 , GNNExplainer would extract three substructures G_{sub1} , G_{sub2} , G_{sub3} that have been determined to contribute significantly (influential) towards the target red-color node prediction while also being present in both graphs from the training dataset (frequented).

Our approach thus focuses on analyzing GNNs over input graphs that we have knowledge about (through the extracted influential substructures). The better the sample of graph inputs we have, the larger and more accurate set of influential substructures we learn—this leads to larger classes of supported graphs. Just as with most DNNs, sources of obtaining training samples vary, e.g., public benchmarks. If available, we can also reuse input graphs that were used to train the GNN models we are analyzing.

2.2 Structure Predicates and Graph Isomorphism

Many existing DNNs and program analyses encode problems into logical formulae that can be reasoned about using constraint solving. Here, we encode the obtained graph substructures as logical predicates σ_{struct} , so that we can leverage existing automating reasoning tools such as SAT and SMT solvers. An important use for these *structure predicates* is to check if an input graph contains the considered substructures. If it does, we are confident that our approach and result will hold; and if it does not, we can support it by adding it to our training data to learn about its influential substructures. These predicates are also a crucial part of the inferred properties that help explain the behaviors of the GNN to the user.

To determine if an input graph satisfies a substructure, we check if the graph and the substructure, which is also a graph, is *isomorphic*. By adapting existing work such as CFL-match [1], we can apply logical reasoning over the obtained structure predicates to check if there exist a mapping from the querying substructure graph to some subgraph of input graph that would make both graphs isomorphic.

Fig. 1 shows these steps. For each obtained substructure, we create a predicate capturing that structure by using standard graph isomorphic checking. As an example structure predicate ensuring present of G_{sub1} which has three nodes x_0 (green), x_1 (blue) and y (red) to be matched to input graph G = (V, E) where V is the set of nodes and E is the set of edges, can has the following form (note that we have omitted node-label checking for readability):

$$\sigma_{struct,sub1}(V, E) = \exists x_0, x_1, y \in V : \{(x_0, x_1), (x_0, x_1), (x_0, y)\} \subseteq E$$
(1)

Concerning the implementation side, this can be done with existing analysis tools by transforming from a graph problem to âa satisfiability problem (e.g., nodes represented as boolean variables and edges as logical connections among variables). Notice if we perform graph isomorphism checking on some input graph such as G_1 in the Figure 1, we will see that it is isomorphic to the predicate of substructure G_{sub1} because they share the same substructure.

Obviously, all trained input sets would be isomorphic to at least one of the structure predicates.

2.3 GNN Unrolling

After obtaining influential substructures and their corresponding substructural predicates, we are now ready to create an FFNN to represent the GNN model. As it turns out, it is actually straightforward to convert a GNN with a fixed substructure directly to an FFNN. We assume our GNN uses the the popular *message passing process*[4] adopted in most types of GNNs. This process works by updating the value of a node in the graph based on the information of its neighboring nodes. Then, to create an FFNN from a GNN with a set of substructures, we essentially create a FFNN to simulate how message passing is done on a substructure using the "unroll" technique similar to one introduced in [7] for RNN unrolling. Finally, we combine all FFNNs to obtain a final FFNN representing the original GNN (that supports graph inputs isomorphic to the considered substructures).

Figure 2 shows how message passing works on the substructure G_{sub1} obtained in Fig. 1. Again, G_{sub1} consists of 3 nodes x_0, x_1 and y, for illustration purposes, we use a GNN with 2-layer and the weight W to represent the values of features of each node. For layer 1, the GNN contains three message passing processes labelled (1), (2), (3) that correspond to the three nodes y, x_1 , and x_0 . The results of these message passing processes are updated as newly computed node features of y, x_1 and x_0 , which are used for next layer. For final layer 2, we only need to consider target node y's message passing from the result of (1), (2) (3), followed by a simple linear transformation and we have a message processing process labeled (4) in Figure 2.

Now, we unroll each message passing process in layer i of the GNN into a corresponding i-layer FFNN. For the three messagepassing processes in Layer 1 in Figure 2a, we obtain the three 1-layer FFNNs shown in Figure 2b and for the message passing process in layer 2 in Figure 2a, we have the 2-layer FFNN shown in Figure 2b (4). Finally, we connect these individual FFNNs to construct a final (large) FFNN as shown in Figure 2b to represent the original GNN.

Using Existing FFNN analyses. We can apply existing analyses for FFNNs to our rolled out FFNN. For instance, we can apply the Prophecy tool [5] to infer properties for FFNNs. This work derives predicates over the inputs of an FFNN, which convex regions over inputs values, that map to a desired output classification. We can also apply FFNN verification tools such as Marabou (the successor of the popular Reluplex work [8]) to check if an inferred or usersupplied property is correct.

For the running example in Figure 2, given some specific weights in Figure 2a, running Prophecy on the resulting FFNN can gives the following predicates representing a convex region over the inputs space that result in the desired classification of the target node in the GNN. Here the input $x_{i,j}$ of the FFNN represents the feature j ICSE 2022, May 21-29, 2022, Pittsburgh, PA, USA

Thanh-Dat Nguyen, Thanh Le-Cong, ThanhVu H. Nguyen, Xuan-Bach D. Le, and Quyet-Thang Huynh

of node x_i of the GNN.

$$\sigma_{inps} = (x_{0,0} + x_{1,0} - x_{0,1} - x_{1,1} > 0)$$

$$\wedge (x_{0,0} + x_{1,0} - 2x_{0,1} - 2x_{1,1} \le 0)$$

$$\wedge (x_{0,0} - x_{0,1} > 0) \wedge (x_{0,0} - 2x_{0,1} > 0)$$

$$\wedge (x_{0,0} + x_{1,0} + x_{2,0} - x_{0,1} - x_{1,1} - x_{2,1} > 0)$$

$$\wedge (x_{0,1} + x_{1,1} + x_{2,1} - 2x_{0,0} - 2x_{1,0} - 2x_{2,0} \le 0)$$
(2)

2.4 Equivalent Analysis

Ideally, the mined influential substructures truly represent the behaviors of the considered GNN and the obtained FFNN is thus equivalent to the GNN. In practice, this does not happen as many nodes, especially those that are not part of the influential substructures but are neighbors with those in the substructure, can influence the final GNN classification result. Thus, we want to analyze how these neighboring nodes can directly affect those in the influential substructures and thus the final result.

Our experiences with GNNs show that a node in a influential substructure is affected by their "outside" neighbors (those that are not in the substructures) in two ways: the number of outside neighbors it has comparing to its total number of neighbors (**connectivity ratio**) and the **mean contribution** of the outside neighbors.

Given this knowledge, we compute additional conditions over substructures to make them represent the GNN more accurately. To do this, we use decision trees to compute predicates over the two features representing connectivity and mean contribution. We split the input graphs (e.g., used in the beginning to obtain substructures) into those that are and are not isomorphic to the substructures. With respect to each influential substructure, we collect the supporting input graph set from the training dataset. Following this, for each input in the supporting graph set, we perform two predictions of target node y's output: 1) using only the influential substructure and 2) using the full input graph. We collect statistics on **connectivity ratio** and **mean contribution** to predict whether the output on target node y remains the same throughout two scenario.

Using this set of training data, we can leverage decision tree to determine conditions over the two features representing connectivity ratio and mean contribution that lead to equivalent or non-equivalent classification. Each paths in the tree represents an additional predicate that can help strengthen the substructures, allowing them to represent the GNN more accurately.

For example, the decision tree in Fig. 3 produces several predicates such as

$$\sigma_{feat \ equiv} := c_0 > 0.2 \land c_1 \le 0.5 \land \bar{x}_{o_1,0} < 0.2, \tag{3}$$

which says that node 0 with connectivity ratio > 0.2, node 1 with connectivity ratio <= 0.5, and the mean contribution of feature 0 in node 0 \geq 0.2 are likely needed as conjunction for the feature predicate on the substructure holds for all graphs. Thus, this approach allows us to obtain a set σ_{inps} of predicates to strengthen the substructure predicates, ensuring they represent the GNN more accurately.

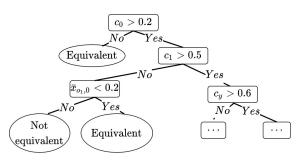


Figure 3: Example of using decision tree to predict whether substructure computation will be equivalent to the input graphs

2.5 GNN Property

 σ

At the end, our approach produces a *property* σ of a given GNN in form of

$$struct\sigma \wedge \sigma_{inps} \wedge \sigma_{feat\ equiv} \Longrightarrow Q$$

where σ_{struct} is predicate capturing graph isomorphism (Section 2.2), σ_{inp} are input properties of the converted FFNN (Section 2.3), σ_{feat_equiv} is the additional constraints helping the FFNN more accurate to the original GNN (Section 2.4), and Q is the output property of some target node y (e.g. $o_{y,1} < o_{y,2}$). This means for an an input graph with target node y that is isomorphic to some of the mined substructure (satisfies σ_{struct}), has certain requirements about neighboring substructure nodes (satisfies σ_{feat_equiv}), with node features lie within certain regions (satisfies σ_{inps}), then this graph will have the property Q on its target node.

3 FUTURE PLAN

Currently, we only have worked out our idea on several small examples by hand. We are now moving to implementing these ideas to automate the process. After that, we will evaluate the approach with existing GNN benchmarks.

We anticipate several challenges that would arise in this direction. First, for complex GNNs, the converted FFNNs might be too complex and contain non-trivial, e.g., nonlinear-arithmetic. These would give difficulties to standard FFNN verification tools such as Reluplex. Second, we use sample inputs to mine substructures and feature predicates, and thus can obtain inaccurate results. While we might be able to obtain "groundtruths" or manually check results of small GNNs, we will not have an effective way to formally verify our results on complex and real-world GNNs. Third, obtaining realistic benchmarks for GNNs might be more difficult as they are not as abundent and well-studied as benchmarks of FFNNs. However, we can start with existing dataset from the literature such as those from [13] for autnomous driving and [4, 20] for drug interactions.

Finally, there is always a chance that this entire approach does not work well in practice, e.g., it does not scale or becomes too inaccurate for converting complex GNNs. It might be that designing algorithms directly to solve GNN would give more benefits in the long run. However, as with any research problem, especially those with few existing attempts, we have to start somewhere, and Toward the Analysis of Graph Neural Networks

converting it to something we do know how to do well seems to be a good place to start.

REFERENCES

- [1] Fei Bi, Lijun Chang, Xuemin Lin, Lu Qin, and Wenjie Zhang. 2016. Efficient subgraph matching by postponing Cartesian products. Proceedings of the ACM SIGMOD International Conference on Management of Data 26-June-20 (2016), 1199–1214. https://doi.org/10.1145/2882903.2915236
- [2] Mark Cheung and José MF Moura. 2020. Graph Neural Networks for COVID-19 Drug Discovery. In 2020 IEEE International Conference on Big Data (Big Data). IEEE, 5646-5648.
- [3] Hanjun Dai, Hui Li, Tian Tian, Xin Huang, Lin Wang, Jun Zhu, and Le Song. 2018. Adversarial attack on graph structured data. In *International conference on machine learning*. PMLR, 1115–1124.
- [4] Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. 2017. Neural Message Passing for Quantum Chemistry. (4 2017). http: //arxiv.org/abs/1704.01212
- [5] Divya Gopinath, Hayes Converse, Corina S. Pasareanu, and Ankur Taly. 2019. Property Inference For Deep Neural Networks. 2019 34th IEEE/ACM International Conference on Automated Software Engineering (ASE) (4 2019), 797–809. https: //doi.org/10.1109/ASE.2019.00079
- [6] Kang-Lin Hsieh, Yinyin Wang, Luyao Chen, Zhongming Zhao, Sean Savitz, Xiaoqian Jiang, Jing Tang, and Yejin Kim. 2020. Drug repurposing for covid-19 using graph neural network with genetic, mechanistic, and epidemiological validation. *Research Square* (2020).
- [7] Yuval Jacoby, Clark Barrett, and Guy Katz. 2020. Verifying Recurrent Neural Networks using Invariant Inference. Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics) 12302 LNCS (4 2020), 57–74. https://doi.org/10.1007/978-3-030-59152-6{_}3
- [8] Guy Katz, Clark Barrett, David L Dill, Kyle Julian, and Mykel J Kochenderfer. 2017. Reluplex: An efficient SMT solver for verifying deep neural networks. In International Conference on Computer Aided Verification. Springer, 97–117.
- [9] Dongsheng Luo, Wei Cheng, Dongkuan Xu, Wenchao Yu, Bo Zong, Haifeng Chen, and Xiang Zhang. 2020. Parameterized Explainer for Graph Neural Network. Advances in Neural Information Processing Systems 33 (2020).
- [10] Ekagra Ranjan, Soumya Sanyal, and Partha Pratim Talukdar. 2019. ASAP: Adaptive Structure Aware Pooling for Learning Hierarchical Graph Representations.

(11 2019). http://arxiv.org/abs/1911.07979

- [11] Pritam Saha, Debadyuti Mukherjee, Pawan Kumar Singh, Ali Ahmadian, Massimiliano Ferrara, and Ram Sarkar. 2021. GraphCovidNet: A graph neural network based model for detecting COVID-19 from CT scans and X-rays of chest. *Scientific Reports* 11, 1 (2021), 1–16.
- [12] Simon Vandenhende, Stamatios Georgoulis, Wouter Van Gansbeke, Marc Proesmans, Dengxin Dai, and Luc Van Gool. 2020. Multi-Task Learning for Dense Prediction Tasks: A Survey. (2020), 1–20. http://arxiv.org/abs/2004.13379
- [13] Xiaolong Wang, Yufei Ye, and Abhinav Gupta. 2018. Zero-shot recognition via semantic embeddings and knowledge graphs. In Proceedings of the IEEE conference on computer vision and pattern recognition. 6857–6866.
- [14] Huijun Wu, Chen Wang, Yuriy Tyshetskiy, Andrew Docherty, Kai Lu, and Liming Zhu. 2019. Adversarial Examples for Graph Data: Deep Insights into Attack and Defense. In Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI-19. International Joint Conferences on Artificial Intelligence Organization, 4816–4823. https://doi.org/10.24963/ijcai.2019/669
- [15] Rex Ying, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. 2019. GNNExplainer: Generating Explanations for Graph Neural Networks. (3 2019). https://arxiv.org/abs/1903.03894
- [16] Rex Ying, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L Hamilton, and Jure Leskovec. 2018. Graph convolutional neural networks for web-scale recommender systems. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 974–983.
- [17] Yadi Zhou, Fei Wang, Jian Tang, Ruth Nussinov, and Feixiong Cheng. 2020. Artificial intelligence in COVID-19 drug repurposing. *The Lancet Digital Health* (2020).
- [18] Dingyuan Zhu, Ziwei Zhang, Peng Cui, and Wenwu Zhu. 2019. Robust graph convolutional networks against adversarial attacks. In Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. 1399–1407.
- [19] Shixiang Zhu, Alexander Bukharin, Liyan Xie, Mauricio Santillana, Shihao Yang, and Yao Xie. 2021. High-resolution Spatio-temporal Model for County-level COVID-19 Activity in the US. ACM Transactions on Management Information Systems (TMIS) 12, 4 (2021), 1–20.
- [20] Marinka Zitnik, Monica Agrawal, and Jure Leskovec. 2018. Modeling polypharmacy side effects with graph convolutional networks. *Bioinformatics* 34, 13 (2018), i457-i466.