

Learning the Satisfiability of Pseudo-Boolean Problem with Graph Neural Networks

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Abstract. Graph Neural Network (GNN) has shown great power on many practical tasks in the past few years. It is also considered to be a potential technique in bridging the gap between machine learning and symbolic reasoning. Experimental investigations have also shown that some \mathcal{NP} -Hard constraint satisfaction problems can be well learned by the GNN models. In this paper, a GNN-based classification model to learn the satisfiability of pseudo-Boolean (PB) problem is proposed. After constructing the bipartite graph representation, a two-phase message passing process is executed. Experiments on 0–1 knapsack and weighted independent set problems show that the model can effectively learn the features related to the problem distribution and satisfiability. As a result, competitive prediction accuracy has been achieved with some generalization to larger-scale problems. The studies indicate that GNN has great potential in solving constraint satisfaction problems with numerical coefficients.

Keywords: Pseudo-Boolean Problem \cdot Graph Neural Network \cdot Constraint satisfaction problem \cdot Deep learning.

1 Introduction

Machine learning, especially deep learning, has shown great power over the past few years. Deep learning systems have dramatically improved the stateof-the-art standards of many tasks across domains, such as computer vision, natural language processing, speech recognition and drug discovery [15]. The tremendous success of deep learning has also inspired us to apply learning-based approaches to solve constraint satisfiability problems (CSPs). There is an interesting prospect that the end-to-end neural network models may have the ability to capture the specific structures of the problem from a certain distribution,

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H. Simonis (Ed.): CP 2020, LNCS 12333, pp. 885–898, 2020. https://doi.org/10.1007/978-3-030-58475-7_51

so that some effective implicit heuristics may be learned automatically. Some previous works have implemented different (deep) neural network architectures to represent such problems and try to learn full-stack solvers [23, 26]. Thanks to the latest progress in graph representation learning, it is promising to apply graph neural networks to solve CSPs, because many of them have topology characteristics, which can be naturally represented as graphs. There have been recent efforts trying to set up end-to-end GNN models to solve the Boolean Satisfiability Problem (SAT), one of the most fundamental problems of computer science [22], and the Traveling Salesman Problem (TSP), an important \mathcal{NP} -Hard problem [20]. Experiments suggest that the GNN-based models can effectively learn the structural features of these problems, thereby obtain pretty high accuracy in predicting the satisfiability. Although such models are not yet comparable with the traditional search-based solvers, it may also be useful to combine them with traditional approaches to improve the solving performance. For instance, the GNN-based classifier for the SAT problem *NeuroSAT* has been further explored and observed to have some ability in finding unsatisfiable cores, which has been used to improve the efficiency of modern SAT solvers such as Glucose and Z3 [21]. We believe that, the GNN-based models also have great potential in improving the efficiency of solving CSPs with numerical constraints.

As a natural and efficient mathematical programming model, pseudo-Boolean (PB) problem, which is also known as 0–1 integer programming, has received much attention in a large number of real-world applications for a long time. Nowadays, techniques related to PB problem are crucial in many fields, such as networked data mining, planning, scheduling, transportation, management and engineering [8, 11]. However, research in complexity theory indicates even solving the satisfiability of PB constraints is an \mathcal{NP} -complete problem [12], which means it is hard to find sufficiently effective algorithms on various distributions. The mainstream approaches for PB problem benefit from the development of both Boolean Satisfiability (SAT) and Integer Programming solving techniques [6,25]. It can be found that fundamentally they are based on the backtracking search frameworks, and largely rely on the heuristic strategies designed by experts in specific domains. It is highly probable that PB solving techniques would also benefit from heuristics learned automatically. For the aforementioned reasons, PB problem provides an important setting for investigating the capability of GNN in extracting features of numerical constraints.

In this paper, we investigate the question that whether an end-to-end GNN model can be trained to solve the satisfiability of pseudo-Boolean problem as a classification task. Other than the previous works, our setting is more universally applicable, because various \mathcal{NP} -Hard CSPs can be easily formulated as PB constraints. At first, we adopt some normalization rules to transform different kinds of constraints into normalized form in order to build a weighted bipartite graph, which can be accepted as the input of GNN. The constructed model is basically a concrete implementation of the Message Passing Neural Network [9]. The revised message passing process is applied to update the node embedding vectors involving edge weights iteratively. Finally, the classification result

is produced after a readout phase. Experiments on two well-known \mathcal{NP} -Hard CSPs, 0–1 knapsack and weighted independent set, demonstrate that our model can well converge on different PB problems under some certain distributions, and predict the satisfiability with high accuracy. The trained model can also be extended to predict the problem instances of larger size than those appeared in training set, which indicates that it has some generalization capability. We can summarize our contribution in the following two points:

- We propose a GNN-based model to solve the decision pseudo-Boolean problem. To the best of our knowledge, it is the first end-to-end GNN model for predicting the satisfiability of a general representation of CSPs with numerical constraints. It has been experimentally confirmed to achieve high accuracy on different benchmarks.
- Compared with another GNN model *NeuroSAT* that intends to solve the SAT problem, our model can be seen as a generalization of it. This is because our model not only achieves the same performance on the SAT problem, but also has ability to solve more general PB problems.

The remainder of this paper proceeds by the following parts. Section 2 summarizes some related work. The problem definition and model architecture are introduced in Sect. 3. The data generation method and training configuration are detailed in Sect. 4, with some analysis about the experimental results. Finally, conclusion and future work are discussed in Sect. 5.

2 Related Work

Although the mainstream algorithms for constraint satisfaction and combinatorial optimization problems are based on reasoning and searching algorithms from symbolism, there have always been attempts trying to solve these problems through machine learning techniques. A class of research is aiming to learn effective heuristics under the backtracking search framework and has achieved progress such as [3, 14, 17]. Here, we concentrate on another route: building endto-end neural network models which directly learn CSP solvers. The earliest research work can be traced back to the Hopfield network [10], which has made progress in solving TSP. It is guaranteed to converge to a local minimum, but the computational power is quite limited. Recently, a series of efforts have attempted to train deep learning models with different representations. [26] proposes CSPcNN, a convolutional neural network model, to solve binary CSPs in matrix form. However, the majority of CSPs are non-binary. [23] introduces a sequenceto-sequence neural network called *Ptr-Net.* [4, 18] further review and extend the model. However, the structural information of CSPs may be partially lost when represented as sequential input. Structure2vec [13] adds graph embedding technique to the model, while it is still a sequential model which can only output greedy-like solutions. In summary, it is necessary to find more powerful representation models to solve various CSPs.

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Fig. 1. The model for solving decision pseudo-Boolean problem based on graph neural network. The pipeline is as follows: (a) A set of constraints is given as input in which all variables can be assigned True or False, then (b) some normalization rules are applied to transform the constraints into normalized form, which is done by equivalent transformation and removing tautologies. From the normalized constraints we can (c) construct a weighted bipartite graph to represent the topological relationship between variables and constraints. Each node in the graph is represented as an embedding vector, which is updated iteratively through (d) the message passing mechanism. Finally, the model (e) outputs prediction about the satisfiability.

Graph neural network has been considered as a promising deep learning technique operating on graphs. Because of its powerful characterization capability for non-Euclidean structure data, the GNN models have made ground-breaking performance on many difficult tasks such as text classification, relation extraction, object detection, semantic segmentation and knowledge graph mining in recent years [27]. We believe graph is a suitable representation for CSPs. A basic fact is that many of the famous \mathcal{NP} -Hard problems are directly defined on graphs such as TSP, Maximum Clique and Minimum Vertex Cover. There have been some works trying to set up GNN-based models to solve SAT [1, 22], [2,5], Graph Coloring Problem [16] and TSP [20]. Our model is distinct from the previous works in many ways. First, PB problem has the capability to conveniently formulate a larger number of CSPs compared with SAT, GCP and TSP. Although SAT is also a well-known meta-problem, it is not intuitive to translate the problem with numerical constraints into conjunction normal form. Second, PB constraints involve integer coefficients and constant items, while TSP has only one kind of numerical information (edge weights) that needs to be processed. Third, [20] introduces edge embeddings to represent the information about edge weights, which may lead to larger parameter space. Actually it takes around 2,000 epochs to converge on the dataset of graphs while $n \sim \mathcal{U}(20, 40)$ as reported. However, the edge weights are considered in the updating process of node embeddings in our model, therefore the required parameter space and training epochs are relatively reduced.

3 Model Architecture

In this section, we first give a brief introduction to the pseudo-Boolean problem. Next, components of the model are illustrated in detail, including the graph construction, the message passing and the readout phase. The whole pipeline of the model is illustrated in Fig. 1.

3.1 Pseudo-Boolean Problem

Pseudo-Boolean problem is one of the most fundamental problems in mathematical programming. Generally, a PB problem should contain a set of pseudo-Boolean constraints. According to whether there is an objective function to optimize, it may vary slightly in definition, which can be divided into the decision problem and the optimization problem. In this paper, we focus on the decision version, in which all the variables are restricted to **True** or **False**, and all the constraints must be satisfied, with no optimization target given. Here is the formal definition: Given *m* constraints C_1, C_2, \ldots, C_m in the form of $C_i: \sum_{j=1}^n c_{ij}x_j \ge b_i$ where $c_{ij}, b_i \in \mathbb{Z}$, decide if a set of assignment to $x_i \in \{0,1\}$ $(1 \le i \le n)$ exists so that all the constraints are satisfied.

The decision PB problem is worthy of investigation for many reasons. Firstly, the bounded integer variables in linear programming can always be expressed as a combination of 0–1 variables by [24]. Moreover, the decision problem can be extended to the optimization version through simple binary search. In terms of complexity, actually it has been proven to be a famous \mathcal{NP} -Complete problem.

3.2 Graph Construction

There have been a series of works trying to apply GNN models to solve constraint satisfaction and combinatorial optimization problems. A critical step is to set up appropriate graph structures for them. [22] characterizes SAT formulas through undirected bipartite graphs, where each literal and clause corresponds to a node and each affiliation relation between literal and clause corresponds to an edge. This kind of representation is quite intuitive and reasonable with at least two justifications. First, it holds the invariance of problem in permutation and negation through graph isomorphism. Second, it imitates the order of reasoning in traditional solving techniques through the message passing process.

For PB problem, we would like to propose a bipartite graph structure which is similar to the previous work. However, the problem structure of PB is quite different from that of SAT in many ways. For instance, the coefficients of PB constraint are arbitrary integers, which cannot be represented in unweighted bipartite graph like *NeuroSAT* does. Besides, non-zero constant terms b_i may exist in PB problem. A question is how to deal with these constant terms in graph construction. Considering the differences above, we propose a two-stage graph construction method.

Constraint Normalization. Given a set of PB constraints, where each constraint $C_i: \sum_{j=1}^n c_{ij}x_j \ge b_i$ where $c_{ij}, b_i \in \mathbb{Z}$, the goal is to transform them into a canonical expression. To achieve this, for a constraint C_i we first replace $c_{ij}x_i$ with $c_{ij}(1-\overline{x_i})$ when $c_{ij} < 0$, and move the constant item to the right side. We denote the resulting constraint $C'_i: \sum_{j=1}^n |c_{ij}||_{x_j} \ge b'_i$, where $l_{x_j} \in \{x_j, \overline{x_j}\}$.

Later we check if the constant item $b'_i > 0$, otherwise the constraint can be removed without changing the satisfiability. Finally we divide both sides of the constraint by b'_i . After the process, all constraints are in normalized form

$$C'_{i}: \sum_{j=1}^{n} c'_{ij} l_{x_{j}} \ge 1$$
 (1)

where $c'_{ij} \in \mathbb{R}^+$ and $l_{x_j} \in \{x_j, \overline{x_j}\}$.

Graph Generation. After the normalization stage above, every constraint C_i $(1 \leq i \leq m)$ in a PB problem is turned into normalized form C'_i or removed from the problem. For each variable x_j $(1 \leq j \leq n)$, we set up a pair of nodes to represent x_j and $\overline{x_j}$ respectively, so we have a total of 2n nodes for variables. Then we set up m nodes for constraints. Suppose a constraint C'_i contains l_{x_j} with the coefficient c'_{ij} , an edge connecting the nodes for C'_i and l_{x_j} is set up if $c'_{ij} \geq 0$ with the weight of c'_{ij} .

3.3 Message Passing

Now a PB problem has been represented as a weighted bipartite graph. The next step is to construct a learning model. We consider the Message Passing Neural Network (MPNN) [9] as the framework. Recently, MPNN has shown its effectiveness in solving some famous combinatorial problems, such as SAT [22] and TSP [20]. In this paper, we propose an MPNN-based model which is fit for PB problem. The forward pass of the model has two phases, a message passing phase and a readout phase.

Message Passing Phase. In the beginning, we parameterize each node in the graph randomly as a *d*-dimensional vector $E_{init} \sim \mathcal{U}(0,1)$ which represents the hidden state. We note the initial hidden states of variables and constraints as $V^{(0)}$ and $C^{(0)}$ respectively. Let M be the adjacency matrix of the bipartite graph defined in the graph generation paragraph above. S is a transformed representation of the relevant nodes which aims to keep the consistency of node embeddings representing the same variable. In this phase, the message passing process runs for T time steps and the hidden states are updated iteratively according to:

$$C^{(t+1)}, C^{(t+1)}_{h} = \mathbf{C}_{\mathbf{u}}(M\mathbf{V}_{\mathbf{msg}}(V^{(t)}), C^{(t)}_{h})$$

$$V^{(t+1)}, V^{(t+1)}_{h} = \mathbf{V}_{\mathbf{u}}(M^{\top}\mathbf{C}_{\mathbf{msg}}(C^{(t)}), V^{(t)}_{h}, S^{(t)})$$
(2)

In the above rules, $\mathbf{C}_{\mathbf{msg}}$ and $\mathbf{V}_{\mathbf{msg}}$ are two message functions implemented with multilayer perceptrons (MLP). Besides, $\mathbf{C}_{\mathbf{u}}$ and $\mathbf{V}_{\mathbf{u}}$ are two updating functions implemented with LSTM networks, where all $C_h^{(t)}$ and $V_h^{(t)}$ are the hidden cell states of LSTM.

Readout Phase. After T iterations of message passing, we apply a readout function $\mathbf{V}_{\mathbf{vote}} : \mathbb{R}^d \to \mathbb{R}^1$ (implemented with MLP) to compute the score that

every variable node votes for the satisfiability of the problem instance. Then we average all the scores to obtain the final result:

$$\hat{y} = mean(\mathbf{V_{vote}}(V^{(T)})) \tag{3}$$

The model is trained to minimize the sigmoid binary cross-entropy loss between \hat{y} and the real satisfiability of the problem instance $\phi(P) \in \{0, 1\}$.

4 Experimental Evaluation

In order to evaluate the performance of our GNN-based model on PB problem, we prepare two different problems for the experiments: 0-1 knapsack problem (0-1KP) and weighted independent set problem (WIS). The above two problems have exceedingly different structures when expressed as PB formulas, whether in terms of the number or the average length of constraints. We generate random datasets for these problems, and train the model on them respectively.

4.1 Data Generation

There are three steps for generating the datasets:

Step 1. Original instances are randomly created following some certain distributions. The number of items in 0-1KP and the number of nodes in WIS are denoted as n. For each problem we uniformly generate several subsets as training sets, each of which contains 100 K instances, with different range of n. Then two datasets are generated in the same way as validation and testing sets, each of which has 10 K instances. Therefore the size ratio of training, validation and testing set is 10:1:1.

Step 2. Because the generated instances are all optimization problems, for each instance we first call *CPLEX* to obtain its optimal solution ϕ , and then randomly choose an integer offset δ from [-R/10, R/10] (*R* is an integer representing the range of coefficients, and we set R = 100 in all experiments). Finally, let $\phi + \delta$ be a bound (i.e. the constant *V* in 0–1KP and *W* in WIS) to completely transform the original instance into a decision problem. It is easy to find that satisfiable and unsatisfiable instances should account for about half of each.

Step 3. The instances are formulated as PB constraints, normalized and turned into graphs through the rules described in Sect. 3. After that the datasets can be fed into the neural network as input for training.

0–1 Knapsack Problem. The 0–1 knapsack problem (KP) is well-known in combinatorial optimization field with a very simple structure: Given a group of items, each with a weight w_i and a value v_i . There is also a backpack with a total weight limit C. The goal is to choose some items to put into the backpack, so that the sum of their values is maximized, and the sum of their weights is not exceeding the given limit of the knapsack. It is proved that the decision problem of 0–1KP is \mathcal{NP} -Complete, so there is no known polynomial-time solving algorithm. It can be naturally represented by the following PB formulas:

$$\sum_{i=1}^{n} w_i x_i \le C$$

$$\sum_{i=1}^{n} v_i x_i \ge V$$
(4)

The constant V represents a bound of the optimal objective. Variable $x_i \in \{0, 1\}$ indicates if an item is put into the backpack.

There have been some research works on generating difficult benchmarks of 0-1KP. Pisinger [19] proposes some randomly generated instances with multiple distributions to demonstrate that the existing heuristics can not find good solutions on all kinds of instances. The four kinds of distributions are named as:

- Uncorrelated: w_i and v_i are randomly chosen in [1, R].
- Weakly correlated: w_i is randomly chosen in [1, R], and v_i in $[w_i R/10, w_i + R/10]$ such that $v_i \ge 1$.
- Strongly correlated: w_i is randomly chosen in [1, R], and $v_i = w_i + R/10$.
- Subset sum: w_i is randomly chosen in [1, R], and $v_i = w_i$.

We generate the datasets of 0–1KP under the above distributions with equal probability. As for the capacity of knapsack C, it is also randomly selected in range $[1, \sum_{i=1}^{n} w_i]$ independently in each instance, in order to ensure sufficient data diversity.

Weighted Independent Set Problem. Given an undirected graph with a weight for each node, an independent set is defined as a set of nodes where any two of them are not connected with an edge. Then the maximum weighted independent set (MWIS) requires the total weights of the selected nodes to be maximized. We can model the decision problem of MWIS as PB formulas:

$$\sum_{i=1}^{n} w_i x_i \ge W$$

$$x_i + x_j \le 1, \ \forall (i,j) \in E$$
(5)

The constant W is a bound of the optimal objective, and the variables $x_i \in \{0, 1\}$ indicates whether each node is selected into the independent set.

To generate the dataset, random graph instances are sampled from the Erdős–Rényi model G(n, p) [7]. The model contains two parameters: the number of nodes n, and the existence probability p of an edge between every pair of nodes. We set p = 0.5 while generating the dataset, which corresponds to the case where all possible graphs on n nodes are chosen with equal probability.

4.2 Implementation and Training

In order to examine the model's capability to predict the satisfiability of PB problem, we implement the model in Python, and several experiments are designed to train the model and evaluate its performance on different datasets for different purposes. All the experiments are running on a personal computer with Intel Core i7-8700 CPU (3.20 GHz) and NVIDIA GeForce RTX 2080Ti GPU.

For reproducibility, we would like to give the setting of hyper-parameters as follows. In our configuration, The dimension of node embedding vectors d = 128, and the time step of message passing T is set to 5 for 0–1KP and 50 for WIS. Our model learns from the training sets in batches, with each batch containing 12 K nodes. The learning rate is set to 2×10^{-5} .

4.3 Experimental Results

Classification Accuracy. As previously noted, the most direct and important target of the model is to classify the satisfiability of PB problems. So we examine it as the first step. There are 7 groups of experiments in total with different settings. For 0-1KP, we set up 3 groups of experiments with different sizes, where n is uniformly distributed in range [3, 10], [11, 40] and [41, 100] respectively. For WIS, we set up 4 groups of experiments with different sizes, where n is uniformly distributed in range [3, 10], [11, 20], [21, 30] and [31, 40] respectively. The reason for lacking of the results in n > 40 is that for each instance the number of constraints is proportional to n^2 , so the graph is too hard to be fully trained in no more than 1,000 epochs. The complete experimental configuration and classification accuracy on the validation and testing sets are shown in Table 1. The first part is the description of datasets, which includes the number of variables, the average number and length of constraints. The constraint length means the number of variables with coefficients other than 0 in a constraint. The number of epochs required for training to convergence is different from each other, and we list the actual spent epochs. Finally, the classification accuracy on the validation and testing sets are shown respectively.

Droblom	#Variables			PB Cons.		Fracha	Accuracy	
Froblein	Train	Valid	Test	$\overline{\#Cons.}$	\overline{Length}	Epocus	Valid	Test
0–1KP	[3,10]	10	10	2.0	6.5	400	86.6%	86.1%
	[11, 40]	40	40	2.0	25.5	400	87.3%	88.2%
	[41,100]	100	100	2.0	70.5	600	79.3%	79.5%
WIS	[3,10]	10	10	11.3	2.4	400	97.7%	97.9%
	[11, 20]	20	20	59.3	2.2	400	92.1%	93.3%
	[21, 30]	30	30	159.2	2.1	400	89.5%	88.9%
	[31,40]	40	40	309.3	2.1	600	86.0%	85.8%

Table 1. The experimental configuration and the classification accuracy results fortraining our model on different PB problems and scales.

The experimental results show that our model can effectively accomplish the classification task on unknown problems with similar distributions. In each group

of $n \leq 40$, the model can converge and obtain more than 85% accuracy both on the validation set and the testing set. When n is expanded to 100 items in 0-1KP, the accuracy is still up to 79%. From the results, our model is believed to have learned some features related to the satisfiability of problems. Furthermore, it is worth noting that the generated PB instances under these problems have very different distributions, whether in terms of the average number or length of constraints. Therefore, it indicates that the model has wide availability to work on different PB problems without changing the structure. This confirms one of the main advantage of our model: general modeling capability.

Comparison with Other Approaches. As far as we know, the proposed model is the first end-to-end GNN model to solve the satisfiability of PB problem. However, because of the close relationship between PB and SAT, we are interested in the comparison between our model (denoted as PB-GNN) and *NeuroSAT*, a GNN-based model that predicts the satisfiability of SAT formulas. We train these two models on the same problems respectively, each for 200 epochs. To transform PB constraints into SAT clauses of equal satisfiability, we call Minisat+1, a high-performance PB solver that achieves excellent ranks in the PB competition². The accuracy results on the validation sets are shown in Table 2. Due to the inevitable introduction of new variables and clauses in the transformation process, the effect of NeuroSAT is limited by the growth of problem scales. For 0-1KP, the training accuracy on NeuroSAT with the transformed SAT formulas is significantly lower than that of the original problems on *PB-GNN.* And for WIS, when training on the original problems where n > 10, it is almost impossible to converge within 200 epochs. Besides, the accuracy results of NeuroSAT when n = 40 are not available, because each epoch takes more than 2 h, which makes the overall training time unacceptable. The results indicate that *PB-GNN* has achieved better performance on general PB problems with numerical constraints. It is worth mentioning that when dealing with SAT instances, we can easily transform SAT clauses into PB constraints. For example, a clause $l_1 \vee l_2 \vee \cdots \vee l_k$ is equivalent to the constraint $\sum_{i=1}^k l_i \ge 1$. In this case, the message passing process of PB-GNN is almost the same as that of *NeuroSAT*. To confirm this, we train the two models for 200 epochs on two datasets SR(3, 10) and SR(10, 40) respectively as defined in [22]. It can be found that the accuracy of *PB-GNN* and *NeuroSAT* is very close, which means the performance of our model is also comparable with the state-of-the-art model on SAT instances.

Another point of concern is the time spent for solving. The average time costs taken by PB-GNN and CPLEX to solve per instance from the testing sets are counted. Table 2 demonstrates the results in milliseconds. It can be seen that compared with the classic CSP solver CPLEX, our model only takes less than 10% of time to return the prediction of satisfiability. In addition to the lower computational amount of the model, another reason is that the problem instances can be input in batches, and the solving process is accelerated with

¹ http://minisat.se/MiniSat+.html.

² http://www.cril.univ-artois.fr/PB16/.

parallelization. This is not to suggest that our model beats the classic solver in time. After all *CPLEX* is able to work without any pre-training. As a matter of fact, the results inspire us a promising scenario of the model when a large number of similar instances need to be solved with high frequency.

Table	2.	Comparison	of th	e classification	accuracy	and	the	average	solving	time
between	n ou	ır model (<i>PE</i>	GNN) and other ap	proaches.					

Droblom		PB-C	INN		ľ	CPLEX		
Froblein	$\overline{\#Var.}$	$\overline{\#Cons.}$	Acc.	\overline{Time}	$\overline{\#Var.}$	$\overline{\#Clau.}$	Acc.	\overline{Time}
0–1KP	5	2.0	89.7%	0.0462	35.4	137.6	74.0%	9.1191
	10	2.0	87.7%	0.0637	87.8	438.7	69.5%	10.7869
	15	2.0	86.1%	0.0785	142.4	774.7	62.8%	12.1947
	20	2.0	86.5%	0.0843	192.7	1084.5	63.7%	13.7513
	40	2.0	85.2%	0.1252	418.1	2502.8		29.9405
WIS	5	6.0	99.0%	0.2747	26.7	108.4	66.3%	15.1882
	10	23.5	96.4%	0.6946	65.5	345.1	51.0%	15.4741
	15	53.5	95.7%	1.3177	101.0	585.4	51.1%	17.2223
	20	95.9	92.5%	1.9140	136.3	836.2	51.4%	19.7416
	40	390.9	82.1%	5.0624	275.9	1958.4		49.6992
SR	[3,10]	46.8	95.8%	0.6619	[3,10]	46.8	95.5%	11.3243
	[11,40]	151.3	84.3%	2.4096	[11,40]	151.3	85.0%	15.7829

Generalization to Larger Scales. We are also interested in whether the model trained on smaller-scale data can work on larger-scale data. We examine two models, one has been trained for 400 epochs on 0–1KP and the other for 600 epochs on WIS, both of which are on the datasets where $n \in [11, 40]$. For each model, we set up 15 groups of data with $n \in [10, 80]$ in steps of 5. Within each group, 5 testing sets are generated with different offset $\delta = \{\pm 1, \pm 2, \pm 5, \pm 8, \pm 10\}$ as described in Sect. 4.1. The other configuration of data generation is the same as that of validation sets. Such testing data can show more clearly the learning effect and generalization ability of our model on the instances of varying complexity.

Figure 2 shows the change in accuracy when testing our model on the above datasets. On one hand, it is easy to find that the generalization ability is related to the problem structure. For 0–1KP, since the structures of different scales are similar, the accuracy can be maintained relatively well even if the problem instances become larger. But for WIS, a larger-scale instance leads to a more complicated graph. The accuracy drops rapidly outside the training set, because the features learned in low dimensions are more likely to lose effectiveness. On the other hand, the model also achieves different accuracy on the instances generated under different offsets. When $\delta = \pm 10$, the accuracy greater than 80%



Fig. 2. The change in accuracy of the model when predicting the satisfiability of largerscale instances than those appeared in the training sets.

can be kept to n = 65 for 0–1KP and n = 50 for WIS. However, the model fails to learn effective features even on the training sets when $\delta = \pm 1$ on both problems. Eventually, when the number of variables continuously increases, the accuracy is reduced to about 50%, which means it almost becomes a purely random model. To conclude, the experimental results indicate that the generalization performance of the model is affected by both the structure and difficulty of the problem.

5 Conclusion and Future Work

In this paper, we investigate whether a deep learning model based on GNN can solve a general class of CSPs with numerical constraints: the Pseudo-Boolean problem. More specially, the target is to correctly classify whether a decision PB problem is satisfiable. We present an extensible architecture that accepts a set of PB constraints with different lengths and forms as input. First, a weighted bipartite graph representation is established on the normalized constraints. After that, an iterative message passing process is executed. Finally, the satisfiability is calculated and returned through a readout phase. Experiments on two representative PB problems, 0–1 knapsack and weighted independent set, show that our model *PB-GNN* can successfully learn some features related to the structure of specific problem within 600 epochs, and achieves high-quality classification results on different distributions. Our model is shown to have several advantages over the previous works. In the aspect of network structure, it integrates the edge weights into the updating function of node embeddings, so that the parameter space is relatively small, making our model easier to converge. Regarding the accuracy of prediction, *PB-GNN* outperforms *NeuroSAT*, a foundational model in this field, on PB benchmarks with numerical coefficients, and is still comparable with it when applied to SAT instances.

We hope the model can provide a basis for a series of future works on learning to solve different CSPs with numerical constraints. There are also several perspectives for further work. On one hand, it needs to be acknowledged that the scale of learnable benchmarks by the current model is relatively small, and it should be improved to learn larger-scale instances, even those benchmarks that are difficult for the state-of-the-art solvers. On the other hand, we will try to decode the assignment of variables from the trained model, so that it can be called a real "solver". There are reasons to believe that the development of graph representation learning will help the model to obtain more accurate features related to the problem structures, thereby reducing the heavy manual work of designing specific heuristic algorithms.

Acknowledgement. This work has been supported by the National Natural Science Foundation of China (NSFC) under grant No. 61972384 and the Key Research Program of Frontier Sciences, Chinese Academy of Sciences under grant number QYZDJ-SSW-JSC036. The authors would like to thank the anonymous reviewers for their comments and suggestions. The authors are also grateful to Cunjing Ge for his suggestion on modeling the problem.

References

- 1. Amizadeh, S., Matusevych, S., Weimer, M.: Learning to solve circuit-SAT: an unsupervised differentiable approach. In: 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA (2019)
- Amizadeh, S., Matusevych, S., Weimer, M.: PDP: a general neural framework for learning constraint satisfaction solvers. arXiv preprint arXiv:1903.01969 (2019)
- Balunovic, M., Bielik, P., Vechev, M.T.: Learning to solve SMT formulas. In: Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems, NeurIPS 2018, Montréal, Canada, pp. 10338–10349 (2018)
- Bello, I., Pham, H., Le, Q.V., Norouzi, M., Bengio, S.: Neural combinatorial optimization with reinforcement learning. In: 5th International Conference on Learning Representations, ICLR 2017, Workshop Track Proceedings, Toulon, France (2017)
- Cameron, C., Chen, R., Hartford, J.S., Leyton-Brown, K.: Predicting propositional satisfiability via end-to-end learning. The Thirty-Fourth AAAI Conference on Artificial Intelligence, AAAI 2020, NY, USA, New York, pp. 3324–3331 (2020)
- Elffers, J., Nordström, J.: Divide and conquer: towards faster pseudo-Boolean solving. In: Proceedings of the Twenty-Seventh International Joint Conference on Artificial Intelligence, IJCAI 2018, Stockholm, Sweden, pp. 1291–1299 (2018)
- Erdős, P., Rényi, A.: On the evolution of random graphs. Publ. Math. Inst. Hung. Acad. Sci 5(1), 17–60 (1960)
- 8. Gass, S.I.: Linear programming: methods and applications. Courier Corporation, North Chelmsford (2003)
- Gilmer, J., Schoenholz, S.S., Riley, P.F., Vinyals, O., Dahl, G.E.: Neural message passing for quantum chemistry. In: Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, pp. 1263–1272 (2017)
- Hopfield, J.J., Tank, D.W.: Neural computation of decisions in optimization problems. Biol. Cybern. 52(3), 141–152 (1985)

- Ivanescu, P.L.: Pseudo-Boolean Programming and Applications: Presented at the Colloquium on Mathematics and Cybernetics in the Economy, vol. 9. Springer, Berlin (2006)
- Karp, R.M.: Reducibility among combinatorial problems. In: Proceedings of a Symposium on the Complexity of Computer Computations, New York, USA, pp. 85–103 (1972). https://doi.org/10.1007/978-1-4684-2001-2_9
- Khalil, E.B., Dai, H., Zhang, Y., Dilkina, B., Song, L.: Learning combinatorial optimization algorithms over graphs. In: Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems, NIPS 2017, Long Beach, CA, USA, pp. 6348–6358 (2017)
- Khalil, E.B., Dilkina, B., Nemhauser, G.L., Ahmed, S., Shao, Y.: Learning to run heuristics in tree search. In: Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, IJCAI 2017, Melbourne, Australia, pp. 659– 666 (2017)
- 15. LeCun, Y., Bengio, Y., Hinton, G.: Deep learning. Nature **521**(7553), 436 (2015)
- Lemos, H., Prates, M.O.R., Avelar, P.H.C., Lamb, L.C.: Graph colouring meets deep learning: effective graph neural network models for combinatorial problems. In: 31st IEEE International Conference on Tools with Artificial Intelligence, ICTAI 2019, Portland, OR, USA, pp. 879–885 (2019)
- Li, Z., Chen, Q., Koltun, V.: Combinatorial optimization with graph convolutional networks and guided tree search. Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, Montréal, Canada, pp. 537–546 (2018)
- Milan, A., Rezatofighi, S.H., Garg, R., Dick, A.R., Reid, I.D.: Data-driven approximations to NP-hard problems. In: Proceedings of the Thirty-First AAAI Conference on Artificial Intelligence, AAAI 2017, San Francisco, California, USA, pp. 1453–1459 (2017)
- Pisinger, D.: Core problems in knapsack algorithms. Oper. Res. 47(4), 570–575 (1999)
- Prates, M.O.R., Avelar, P.H.C., Lemos, H., Lamb, L.C., Vardi, M.Y.: Learning to solve NP-complete problems: a graph neural network for decision TSP. In: The Thirty-Third AAAI Conference on Artificial Intelligence, AAAI 2019, Honolulu, Hawaii, USA, pp. 4731–4738 (2019)
- Selsam, D., Bjørner, N.: Guiding high-performance SAT solvers with Unsat-Core predictions. In: Janota, M., Lynce, I. (eds.) SAT 2019. LNCS, vol. 11628, pp. 336– 353. Springer, Cham (2019). https://doi.org/10.1007/978-3-030-24258-9_24
- Selsam, D., Lamm, M., Bünz, B., Liang, P., de Moura, L., Dill, D.L.: Learning a SAT solver from single-bit supervision. In: 7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA (2019)
- Vinyals, O., Fortunato, M., Jaitly, N.: Pointer networks. Advances in Neural Information Processing Systems 28: Annual Conference on Neural Information Processing Systems, NIPS 2015, Montreal, Quebec, Canada, pp. 2692–2700 (2015)
- Williams, H.P.: Logic and Integer Programming. ISORMS, vol. 130. Springer, Boston, MA (2009). https://doi.org/10.1007/978-0-387-92280-5
- 25. Wolsey, L.A., Nemhauser, G.L.: Integer and Combinatorial Optimization. John Wiley & Sons, Hoboken (2014)
- Xu, H., Koenig, S., Kumar, T.K.S.: Towards effective deep learning for constraint satisfaction problems. In: Hooker, J. (ed.) CP 2018. LNCS, vol. 11008, pp. 588–597. Springer, Cham (2018). https://doi.org/10.1007/978-3-319-98334-9_38
- 27. Zhou, J., et al.: Graph neural networks: a review of methods and applications. arXiv preprint arXiv:1812.08434 (2018)