NeuroSchedule: A Novel Effective GNN-based Scheduling Method for High-level Synthesis

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Abstract

High-level synthesis (HLS) is widely used for transferring behavior-level specifications into circuit-level implementations. As a critical step in HLS, scheduling arranges the execution order of operations for enhanced performance. However, existing scheduling methods suffer from either exponential runtime or poor quality of solutions.

This paper proposes an efficient and effective GNN-based scheduling method called NeuroSchedule, with both fast runtime and enhanced solution quality. Major features are as follows: (1) The learning problem for HLS scheduling is formulated for the first time, and a new machine learning framework is proposed. (2) Pre-training models are adopted to further enhance the scalability for various scheduling problems with different settings. Experimental results show that NeuroSchedule obtains near-optimal solutions while achieving more than **50,000**× improvement in runtime compared with the ILP-based scheduling method. At the same time, NeuroSchedule improves the scheduling results by 6.10% on average compared with state-of-the-art entropy-directed method. To the best of our knowledge, this is the first GNN-based scheduling method for HLS.

1 Introduction

Recently, FPGA has been playing an important role in accelerating computations from the cloud to the edge [1, 2, 3, 4, 5]. As a reconfigurable computing device, FPGA gains increasing popularity for its high performance and great energy efficiency. However, developers are required to write programs using the hardware description language (HDL) to implement applications in FPGAs, which is time-consuming and error-prone. Therefore, the utilization of FPGA's enormous computing power is limited by the cumbersome developing process.

As a result, the concept of high-level synthesis (HLS) is proposed in the EDA community to speed up the developing process [6, 7, 8]. HLS automatically transfers high-level specifications (written in high-level languages like C/C++) to behavior-level implementations (written in HDLs like Verilog/VHDL). Figure 1 presents the whole flow of HLS. As shown in the figure, HLS mainly comprises three parts: compilation, synthesis, and generation. For compilation, high-level languages are transferred to Control Data Flow Graphs (CDFGs) with the assistance of modern compilers like GCC or LLVM. During the synthesis process, hardware resources (e.g. functional units, storage, and wires) are first allocated. According to the allocated hardware resources, the operations in CDFG (such as ADD and MUL) are scheduled to certain time steps. After scheduling, the allocated hardware resources are

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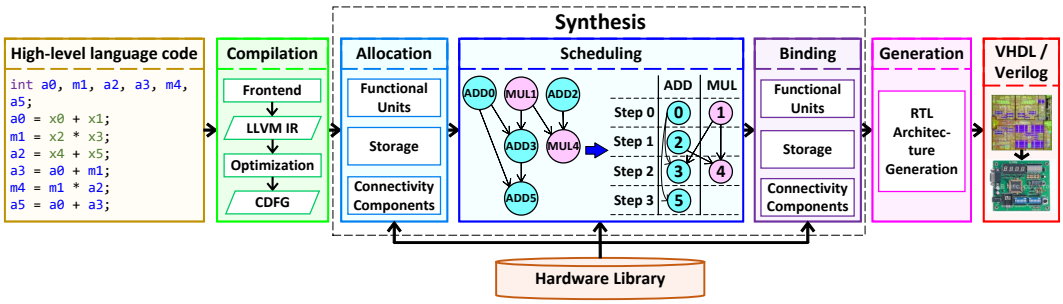

Figure 1: High-level synthesis flow.

bound to corresponding operations and time steps. After synthesis, the generation process generates corresponding HDLs according to the synthesized results.

Scheduling is one of the most critical stages in the HLS process, which arranges the execution order of operations, and thus determines the performance of generated circuits. As depicted in Figure 1, according to the allocated hardware resources and the dependencies between operations, the operations in CDFG are arranged in different time steps. For example, during the scheduling process, operation ADD0 is scheduled to step 0 and bound to the adder. It is noteworthy that only one adder is allocated to the scheduling task. So operation ADD2 could not be scheduled to step 0 same as operation ADD0. Therefore, determining the scheduling priority for the operations is the key objective of the scheduling problem. However, the scheduling problem has been proved to be NP-hard [9]. And existing algorithms suffer from either unbearable long runtime or poor quality of solutions. Integer linear programming (ILP) formulation has been proposed to solve the scheduling problem optimally [10]. However, the exponential runtime of ILP is unbearable. Therefore, various heuristic algorithms are proposed to obtain sub-optimal solutions within acceptable runtime. List scheduling is one of the most famous heuristic algorithms [11]. List scheduling stores ready operations in a list and arranges them according to a heuristically defined priority function. Based on the list scheduling algorithm, force-directed scheduling algorithm is proposed [12], which builds a force-distribution graph for representing the priority function. Inspired by the force-directed scheduling algorithm, Entropy-Directed Scheduling (EDS) algorithm [13] replaces the priority function with the entropy of CDFGs to be scheduled. The utilization of the entropy function not only speeds up the scheduling process, but also improves the quality of solutions. Different from the algorithms in the list scheduling family, an algorithm based on the system of difference constraints (SDC) is proposed to speed up the ILP-based algorithm. SDC-based algorithm transfers the scheduling constraints into a system of difference constraints using heuristics, which greatly reduces the number of equations to be solved. However, the SDC-based algorithm cannot guarantee the optimal solution. Therefore, the aforementioned heuristic algorithms all trade quality of solutions for runtime, which leaves a large optimization space to be explored.

On the one hand, the complicated dependencies of operations in the CDFG bring great challenges to the scheduling process. On the other hand, Graph Neural Networks (GNNs) [14, 15, 16, 17] have great representational power of complicated graphs, which is suitable for extracting complicated relations between operations in CDFGs. Therefore, a natural idea is to adopt GNNs to tackle the scheduling problem for both fast runtime and high-quality solutions. This paper proposes the first GNN-based scheduling algorithm called NeuroSchedule. Inspired by algorithms in the list scheduling family, NeuroSchedule builds a GNN model to predict the priorities of operations in the CDFG. The predicted priorities are then used to arrange the operations in CDFG to obtain the scheduling results. Major contributions of this paper are summarized as follows:

- A learning problem for the HLS scheduling is first formulated, and then a GNN-based learning framework is proposed to effectively and efficiently solve the problem.
- Pre-training models are adopted to further enhance the scalability for different scheduling problems with different settings.
- Experimental results indicate that NeuroSchedule obtains near-optimal solutions while achieving more than **50,000**× speedup compared with the ILP-based algorithm [10]. At the same time, NeuroSchedule improves the scheduling results by 6.10% on average compared with the state-of-the-art EDS algorithm [13].

The rest of this paper is organized as follows. Section 2 gives a motivating example for the GNN-based scheduling method. Section 3 gives preliminaries and the formulation of the GNN-based

scheduling problem. The proposed machine learning framework is presented in Section 4. Section 5.2 introduces NeuroSchedule, as well as the pre-training models adopted for enhancing the scalability. Section 6 presents the experimental results. Finally, conclusion is drawn in Section 7.

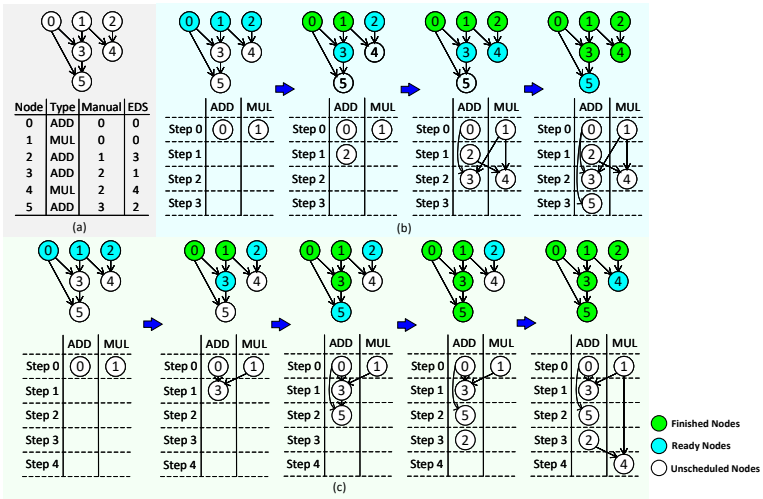

Figure 2: A motivating Example. (a) CDFG and the priority of nodes. (b) Manually designed list scheduling result (4 cycles). (c) Entropy-directed scheduling result (5 cycles).

2 Motivation

As introduced in Section 1, the list scheduling algorithm stores ready operations in a list and schedules them according to a heuristically defined priority function. Here, a ready operation means all of its predecessing operations are finished and the operation could be scheduled for execution immediately. For example, in Figure 2(a), node 3 is ready when node 0 and node 1 are finished. The process of list scheduling could be stated as follows. First, the ready operations are stored in a list. Next, the operation with the highest priority in the list is picked to be scheduled to available hardware resources (e.g. adders and multipliers) for execution. After the operation is finished, the newly generated ready operations are stored in the list. The above process is iterated until all the operations are successfully scheduled. From the list scheduling process, defining precise priority functions is crucial to obtain good scheduling results.

A motivating example is given in Figure 2. Figure 2(a) presents the CDFG to be scheduled, which consists of 6 operations with 2 types (ADD and MUL). And the available hardware resources for scheduling are an adder (for ADD) and a multiplier (for MUL). Figure 2(c) depicts the entropy-directed scheduling process, which takes the entropy function for the priority computation. In the figure, ready operations are colored blue and finished operations are colored green. Since the entropy priority of node 3 is higher than node 2, node 3 is scheduled before node 2. However, scheduling node 3 first delays the scheduling of node 4, which makes the multiplier idle for 3 cycles (i.e. time steps). Consequently, the final scheduling result is not optimal. In Figure 2(b), we assume there is an optimal manually designed priority function. Based on the optimal priority function, node 2 is scheduled before node 3, and thus the hardware resources are fully utilized. Therefore, the scheduling algorithm based on the manual function gives the optimal solution.

The success of the manually designed function motivates us to build a machine learning framework, which learns the priority function automatically. GNNs are an effective framework for representation learning of graphs, which follow a neighborhood aggregation scheme. In GNNs, representation vectors of nodes are computed by recursively aggregating and transforming representation vectors of their neighboring nodes [14]. Therefore, GNNs are suitable to learn the CDFG embeddings for obtaining the priority function. As a result, a GNN-based machine learning framework is proposed to learn the priority function. Experiments verify the effectiveness of the proposed scheduling method based on GNN.

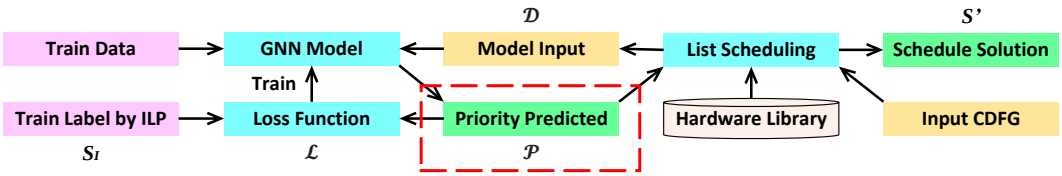

Figure 3: Framework for NeuroSchedule.

3 Preliminaries and Problem Formulation

CDFG. In high-level synthesis, the program in high-level language is first translated into CDFG, a graph-based representation defined as follows:

Definition 1 *A CDFG $G = (V, E)$ is a directed graph with node set V and edge set E. Each node $v \in V$ represents an operation, e.g. add or load. Each directed edge $e = (v_i, v_j) \in E, i, j \in 1, ..., |V|$ represents a dependency relationship between operation v_i and v_j, i.e., operation v_j must be executed after the execution of operation v_i.*

ASAP and ALAP. The As-Soon-As-Possible (ASAP) algorithm and the As-Late-As-Possible (ALAP) algorithm give the information about node flexibility during the scheduling process. For node $v_i \in V$, the result of ASAP and ALAP can be formulated as follows:

$$ASAP(v_i) = \begin{cases} \max ASAP(v_j) + 1 & \exists (v_j, v_i) \in E, v_j \in V \\ 0 & \nexists (v_j, v_i) \in E, v_j \in V \end{cases} \tag{1}$$

$$ALAP(v_i) = \begin{cases} \min ALAP(v_j) - 1 & \exists (v_i, v_j) \in E, v_j \in V \\ \max\limits_{v_k \in V} ASAP(v_k) & \nexists (v_i, v_j) \in E, v_j \in V \end{cases} \tag{2}$$

Resource-constrained scheduling problem. Based on the CDFG, we have to solve the resource-constrained scheduling problem: given the number of resources, find the scheduling solution with the minimum number of execution cycles, while satisfying the given set of scheduling and resource constraints. Given a functional unit set U, where $u_i \in U$ represents a functional unit, such as an adder. Denote d_{u_i} as the cycle delay of functional unit u_i. Given a CDFG $G = (V, E)$, and let $n = |V|$, a *schedule* can be defined as $S = (t_1, t_2, ..., t_n, f_1, f_2, ..., f_n)$, where $\forall i \in 1, 2, ..., n$, (1) $t_i \in \mathbb{N}^*$, denoting the start cycle of operation $v_i \in V$, (2) $f_i \in U$, denoting the functional unit used by operation v_i. Let $L = \max\limits_{i \in 1,...,n} t_i + d_{f_i} - 1$ denote the total number of execution cycles. The resource-constrained scheduling problem minimizes L, which can be defined as follows:

Definition 2 *Find an optimal schedule $S' = (t'_1, t'_2, ..., t'_n, f'_1, f'_2, ..., f'_n)$, such that:*

a) $\forall e = (v_i, v_j) \in E, i, j \in 1, 2, ..., n,\ t'_i + d_{f'_i} \leq t'_j$

b) $\forall i, j \in 1, 2, ..., n, i \neq j,\ f'_i = f'_j \Longrightarrow |t'_i - t'_j| \geq d_{f'_i}$

c) $L = \max\limits_{i \in 1,...,n} t'_i + d_{f'_i} - 1$ *is minimized.*

List scheduling. As introduced in Section 2, list scheduling is an effective scheduling algorithm. It divides the node set V into three sets, finished nodes V_F, ready nodes V_R, and unscheduled nodes V_U. Given the node priority function $\mathcal{F}$, where $\mathcal{F}(v_i) < \mathcal{F}(v_j), v_i, v_j \in V_R$ indicates that operation v_i has a higher priority than operation v_j. At each step, list scheduling algorithm chooses the node $v_h \in V_R$ to schedule, where $\mathcal{F}(v_h) = \min\limits_{v_r \in V_R} \mathcal{F}(v_r)$. A better priority function in the list scheduling algorithm corresponds to a better scheduling solution. As the ILP-based scheduling algorithm can get the optimal scheduling results, the scheduling result $S_I = (t_{I1}, t_{I2}, ..., t_{In}, ...)$ is a good candidate for the priority function, where $\mathcal{F}(v_x) = t_{Ix}, v_x \in V$. However, for large scheduling problems, the runtime of the ILP-based algorithm is not acceptable. Therefore, we propose the GNN model to predict the priority function.

Neural Network Model. Denoting the input data as $\mathcal{D}$, our model can be formulated as:

$$\mathcal{P}(i) = MLP(GIN_EMBED(\mathcal{D}_i)) \tag{3}$$

Our loss function can be formulated as:

$$\mathcal{L} = \mathcal{L}(\mathcal{P}, S_I) \tag{4}$$

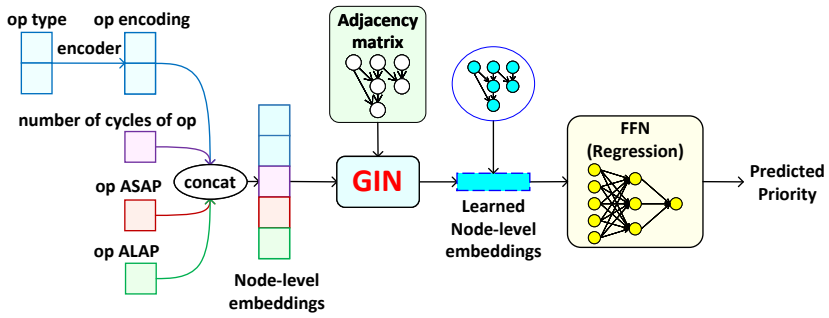

Figure 4: Model Architecture.

Details of our loss function will be introduced in Section 4. Figure 3 shows the framework of our NeuroSchedule algorithm. The ILP-based scheduling algorithm is adopted to generate the training labels for our GNN model. The output of the GNN model, i.e. $\mathcal{P}$, is used by the list scheduling algorithm as the priority function, which obtains significantly enhanced scheduling solution.

4 Model Design

A machine learning framework is proposed to learn the priority function in the list scheduling algorithm. In the proposed framework, the CDFG is taken as input, and a GNN model is trained to predict the priorities of the operations. This section gives the model input, the model architecture, and the selection of loss function.

4.1 Model Input

The input of a GNN model includes an adjacency matrix representing graph connections and a tensor representing node features. Different node features will be selected for different problems. In the scheduling problem, the node features consist of operation type, number of cycles of the operation, along with the above-defined ASAP and ALAP.

Operation's type and number of cycles. As the operation type is categorical and discrete, inspired by the graph-based program representation [18], the operation type is encoded by one-hot encoding. For the number of cycles of an operation, the cycle number is directly used in the encoding. For example, if there are two types of operations (MUL, ADD) and the cycle number of MUL operation is 1, the node feature of MUL operation could be represented as [1, 0, 1]. Here, "10" from the first "1" and second "0" in the feature denotes MUL.

Operation's ASAP and ALAP. Except for operation's type and number of cycles, ASAP and ALAP are also adopted in the node features. As introduced in Section 3, ASAP and ALAP represent the earliest step and the latest step that an operation could be scheduled, respectively. The ASAP and ALAP of an operation indicate the operation's flexibility during scheduling. For example, the ASAP of node ADD2 in Figure 5 is step 0 and the ALAP is step 1, which means node ADD2 could be scheduled between step 0 and step 1. Different from node ADD2, the ASAP and ALAP of node ADD3 in Figure 5 are both step 1, which means node ADD3 could only be scheduled to step 1. The reason why ASAP and ALAP are adopted in the node features is that the flexibility of an operation affects its priority during scheduling. Operations with low flexibility during scheduling tend to be the bottlenecks [13], which should be scheduled with high priority to fully utilize the hardware resources.

Finally, the operation's type, operation's number of cycles, along with normalized ASAP and ALAP, are concatenated as a tensor representing node features. For example, there are two operations in

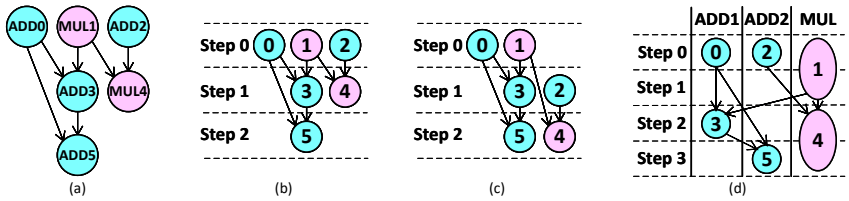

Figure 5: An example for ASAP, ALAP, and multi-cycle operations. (a) The CDFG. (b) The result of ASAP. (c) The result of ALAP. (d) A special scheduling example with multi-cycle operations.

Figure 5, MUL and ADD, and the number of cycles of operations MUL and ADD are both 1. So node ADD3 could be encoded as [0, 1, 1, 0.5, 0.5]. It is noteworthy that the ASAP and ALAP of an operation are normalized according to the maximum ASAP value among all the operations. The normalization is conducted because the number of operations in the CDFG varies such that using the absolute ASAP and ALAP values will bring noises.

4.2 Model Architecture

Figure 4 presents the architecture of the proposed model. As shown in the figure, the proposed model is composed of a GNN model and a feed-forward network (FFN) model. The GNN model is adopted to learn the embedding of each operation from the operation features and graph structure, while the FFN model is utilized to conduct regression tasks for predicting operations' priorities. The workflow of the model is presented as follows. First, operation features including the operation's type, operation's number of cycles, along with normalized ASAP and ALAP are concatenated into a feature tensor as introduced in Section 4.1. Next, a GNN model is adopted to learn operation embedding from the feature tensor and graph structure. Graph Isomorphism Network (GIN) is used as the GNN model for its strong power of learning embeddings from graph structures [14]. Finally, the learned operation embedding is fed into the FFN model for predicting the operations' priorities. In the FFN model, there are three fully-connected layers, and ReLU is adopted as the activation function [19].

4.3 Training Settings

As depicted in Figure 4, the proposed model outputs the operations' priorities by regression. To effectively train the proposed model, a dedicated training pipeline is proposed. The proposed training pipeline mainly focuses on two questions: 1. How to acquire the regression labels; 2. How to select the training objective function (a.k.a loss function).

Training label. As formulated in Section 3, training the priority prediction task requires a collection of data $\mathcal{D} = \{g_i, p_i, c_i\}$, where g_i denotes CDFG's graph structure, p_i denotes operation properties (such as ASAP and ALAP), and c_i denotes the training label. In the proposed training pipeline, the ILP-based method is used to generate the regression labels [10]. The details are presented as follows. The ILP-based method gives the optimal solution, which arranges CDFG's operations into suitable time steps. Obviously, operations arranged in later time steps have lower priorities than those arranged in earlier time steps. Therefore, in the proposed training pipeline, the time step obtained by the ILP-based method (i.e. t_{Ii} in Section 3) is taken as the regression label c_i. As mentioned in Section 4.1, the time step of an operation is also normalized based on the maximum time step, which reduces the impact of noises. Figure 2 gives an example. In the manually designed priority function, the time step could be solved by the ILP-based method. As shown in the figure, the ILP-solved time steps $[0, 0, 1, 2, 2, 3]$ are assigned to corresponding operations. After normalization, the ILP-solved time steps are computed as $[0, 0, 0.33, 0.66, 0.66, 1]$.

Training objective function. The mean square error (MSE) function is commonly adopted for training a regression task. Given dataset $\mathcal{D} = \{g_i, p_i, c_i\}$, the output of our GNN model has the form $\mathcal{P}(i) = \mathcal{P}(g_i, p_i)$. The MSE function $\sum_i (\mathcal{P}(i) - c_i)^2$ guides the model to accurately predict the operations' priorities. However, the scheduling task cares more about the operations' relative order rather than the absolute priority values of the operations. Moreover, it takes more effort for training a model to predict the absolute value than to predict the rank. Therefore, inspired by AutoTVM [20], the following rank loss function is adopted to train the model for predicting the rank of all operations [21]:

$$\mathcal{L} = \sum_{i,j} \log(1 + e^{-\operatorname{sign}(c_i - c_j)(\mathcal{P}(i) - \mathcal{P}(j))}). \tag{5}$$

During training, the above rank loss function keeps the relative order of operations' priorities with reduced training efforts.

5 NeuroSchedule

5.1 Pre-training for Different Scheduling Settings

As introduced in Section 4.1, the input of our model consists of the operation's type and operation's number of cycles, along with normalized ASAP and ALAP. It works well when the numbers of

Algorithm 1 NeuroSchedule algorithm.

Input: Trained network model $\mathcal{P}$, CDFG $G = (V, E)$, functional unit set U, delay array d
Output: Generated schedule $S_{\mathcal{P}}$

1: $V_F \leftarrow \phi, V_R \leftarrow \phi, V_U \leftarrow V, S_{\mathcal{P}} \leftarrow \phi, Time \leftarrow 0$
2: $\mathcal{D} \leftarrow encodeData(G)$
3: $\mathcal{F} \leftarrow runModel(\mathcal{P}, \mathcal{D})$
4: **for** v_i in V **do**
5: **if** $v_i.inDegree() = 0$ **then**
6: $V_R \leftarrow V_R \cup v_i, V_U \leftarrow V_U \setminus v_i$
7: **while** $|V_F| < |V|$ **do**
8: **for** u_j in U **do**
9: $M \leftarrow MAX_FLOAT, v_{chosen} \leftarrow \phi$
10: **for** v_i in V_R **do**
11: **if** $\mathcal{F}(v_i) < M$ **and** $v_i.canUse(u_j)$ **then**
12: $M \leftarrow \mathcal{F}(v_i), v_{chosen} \leftarrow v_i$
13: **if** $v_{chosen} = \phi$ **or** $u_j.unavailable(Time)$ **then**
14: **continue**
15: $S_{\mathcal{P}}.insert(v_{chosen}, u_j, Time)$
16: $u_j.setUnavailable(Time, Time + d_{u_j} - 1)$
17: $V_R \leftarrow V_R \setminus v_{chosen}, V_F \leftarrow V_F \cup v_{chosen}$
18: **for** v_i in V_R **do**
19: **if** $(v_{chosen}, v_i) \in E$ **then**
20: $E \leftarrow E \setminus (v_{chosen}, v_i)$
21: **if** $v_i \in V_U$ **and** $v_i.inDegree() = 0$ **then**
22: $V_R \leftarrow V_R \cup v_i, V_U \leftarrow V_U \setminus v_i$
23: $Time \leftarrow Time + 1$

functional units are fixed. However, there are various scheduling settings in real HLS cases including: (1) different operation types, (2) different number of functional units for each type, and (3) different number of cycles for different operation types. Figure 5(d) gives a scheduling example with 2 adders, 1 multiplexer, and multi-cycle operations, i.e., the MUL operation takes 2 cycles. Therefore, for scheduling problems with different settings, specified GNN models are required to get valid solutions. However, it is infeasible to train a GNN model for each scheduling setting due to the unbearable training efforts. Therefore, we build a dataset of CDFGs with different scheduling settings, and pre-train our model with the dataset. To specify the scheduling setting, we add the number of the corresponding functional units into the node features of each operation. While dealing with a specific scheduling setting, we fine-tune the model using the randomly generated data from the setting. Compared with direct training, the fine-tuning takes fewer efforts with enhanced scheduling solutions.

5.2 NeuroSchedule Algorithm

Algorithm 1 gives an overview of the proposed NeuroSchedule algorithm, which is based on the traditional list scheduling algorithm and our neural network models. The symbols in Algorithm 1 are defined in Section 3. We use trained network model $\mathcal{P}$ as priority function $\mathcal{F}$ (line 3), and run the loop until each node in the CDFG is successfully scheduled (line 7). In each cycle, we try to schedule every available functional unit using the node v_{chosen} with the highest priority. After the node v_{chosen} is selected from the ready set V_R, we update the schedule $S_{\mathcal{P}}$, and the sets V_R and V_F (line 16). Then we delete all the out edges (v_i, v_{chosen}) of v_{chosen} (line 20). If the in-degree of v_i equals 0, we add v_i into the ready set V_R. Finally, the scheduling solution is obtained in $S_{\mathcal{P}}$.

6 Experiments

The proposed GNN-based scheduler is implemented in Python (version 3.9.12), and the GNN model is designed and trained with Pytorch [22] (version 1.8.0) and pyG [23] (version 2.0.4). To train the GNN model, we build a dataset including 50,000 CDFGs. The operations in the CDFGs are annotated with the priorities solved by the ILP-based method (as introduced in Section 4.3). For efficiency, Gurobi [24] is adopted as the ILP solver. Details of dataset preparation are presented in supplementary materials. We conduct all the experiments on a Ubuntu 20.04 LTS Linux Server with a CPU (Intel(R) Xeon(R) Gold 5218 CPU@2.30GHz) and a GPU (NVIDIA Tesla V100). The experiments are conducted to answer the following questions:

Table 1: Results of NeuroSchedule.

Testcase			CDFG size		NeuroSchedule		Entropy-directed		ILP-based		Result	
Dataset	Name	Basic Block	Node	Edge	Cycle	Time	Cycle	Time	Cycle	Time	δ [1]	Imp.[2]
CHStone	adpcm	main	78	174	**52**	0.019	54	0.004	52	2.842	0.00%	3.70%
CHStone	aes	ARK_InvCol	79	192	**77**	0.013	**77**	0.005	77	2.430	0.00%	0.00%
CHStone	blowfish	BF_set_key	147	456	**80**	0.107	81	0.010	80	14.67	0.00%	1.23%
CHStone	dfadd	R&PFloat64	92	238	49	0.013	50	0.005	48	3.570	2.04%	2.00%
CHStone	dfdiv	float64_div	433	1252	**235**	0.060	256	0.027	N/A	$>10^4$	/	8.20%
CHStone	dfmul	float64_mul	339	914	**192**	0.115	207	0.019	N/A	$>10^4$	/	7.25%
CHStone	dfsin	float64_div	392	1187	**203**	0.063	224	0.026	N/A	$>10^4$	/	9.38%
CHStone	gsm	main	68	148	41	0.029	41	0.003	40	2.121	2.44%	0.00%
CHStone	jpeg	write4Blocks	213	692	**127**	0.022	132	0.014	N/A	$>10^4$	/	3.79%
CHStone	mips	main	364	1433	**200**	0.038	**200**	0.025	200	2207	0.00%	0.00%
CHStone	motion	mt_Vectors	25	59	**14**	0.010	16	0.003	14	0.509	0.00%	12.5%
CHStone	sha	final	79	202	**49**	0.012	55	0.004	49	4.141	0.00%	10.9%
MiBench	cosine1	cosine1	66	76	**43**	0.025	44	0.006	43	41.95	0.00%	2.27%
MiBench	cosine2	cosine2	82	91	**57**	0.100	58	0.003	57	11.07	0.00%	1.72%
MiBench	fir1	fir1	44	43	**34**	0.098	**34**	0.002	34	1.244	0.00%	0.00%
MiBench	fir2	fir2	40	39	**31**	0.028	32	0.002	31	1.478	0.00%	3.13%
MiBench	idctcol	dfg_3	114	164	**69**	0.103	**69**	0.004	69	16.22	0.00%	0.00%
MiBench	write	bmp_7	88	202	**68**	0.097	69	0.004	68	5.759	0.00%	1.45%
Total			2761	7448	**1621**	0.952	**1699**	0.167	/	$>5\times10^4$		
Optimal Rate					**88.89%**		**16.67%**		N/A			
Average Improvement											**0.30%**	**6.10%**[3]

[1] δ = (NeuroSchedule - ILP) / ILP.
[2] Improvement = (EDS - NeuroSchedule) / EDS.
[3] Average Improvement = (Σ Cycle_NeuroSchedule - Σ Cycle_ILP) / Σ Cycle_ILP. The optimal solutions (Imp. = 0.00%) are not counted in.

Q1: Could NeuroSchedule obtain better solutions than the entropy-directed algorithm?
Q2: Could NeuroSchedule obtain optimal solutions with respect to the ILP-based method?
Q3: How fast is the proposed algorithm compared against the ILP-based method?
Q4: How do the pre-training methods work in enhancing the algorithm's scalability?
Q5: What are the differences between different loss functions?

6.1 Quality of Solutions

To answer **Q1**, we evaluate the performance of NeuroSchedule against state-of-the-art entropy-directed scheduling algorithm [13] and ILP-based method [10] using the benchmarks from CHStone [25] and MiBench [26]. The experimental results are presented in Table 1. As shown in the table, NeuroSchedule improves the scheduling results by 6.10% on average compared with EDS. Moreover, compared with the ILP-based method, NeuroSchedule obtains optimal solutions in 88.89% of the benchmarks and near-optimal solutions in the rest, while EDS can only obtain 16.67% optimal solutions in all benchmarks.

To answer **Q2**, we synthesize a benchmark suite including large CDFGs with complex dependencies among the operations. The entangled dependencies make it hard for scheduling algorithms to find an optimal solution. We evaluate NeruoSchedule, entropy-directed algorithm [13] and ILP-based algorithm [10] on the synthesized complex benchmark suite. The results are presented in Figure 6. Figure 6 gives the heatmaps for comparing the scheduling results among NeuroSchedule, entropy-directed algorithm, and ILP-based algorithm. As shown in Figure 6(a), NeuroSchedule obtains optimal solutions on 90% of the synthesized complex benchmarks. While in Figure 6(b), the entropy-directed algorithm fails to obtain optimal solutions on all of the benchmarks due to the complex operation dependencies. Moreover, as shown in Figure 6(c), NeuroSchedule obtains better solutions on 94% of the synthesized complex benchmarks compared with the entropy-directed algorithm.

6.2 Execution Time

To answer **Q3**, we evaluate the runtime of NeuroSchedule against state-of-the-art entropy-directed scheduling algorithm and ILP-based method [10] using benchmarks from CHStone [25] and MiBench [26]. The results are presented in Table 1. As shown in the table, NeuroSchedule achieves more than **50,000**$\times$ speedup compared with the ILP-based method, while obtaining near-optimal solutions. Moreover, the ILP-based method fails to solve certain benchmarks within 10,000 seconds due to the exponential runtime overhead. Besides, since NeuroSchedule needs to launch CUDA kernels to compute operation priorities, it runs a little slower than the entropy-directed algorithm.

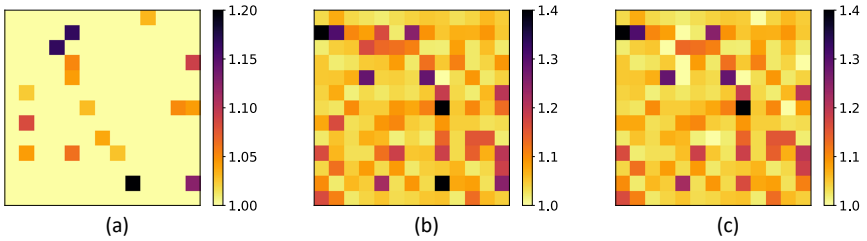

Figure 6: Evaluations on synthesized complex benchmark suite. The values in the heatmaps represent the relative scheduling results between different algorithms. (a) NeuroSchedule relative to ILP-based algorithm. (b) Entropy-directed algorithm relative to ILP-based algorithm. (c) Entropy-directed algorithm relative to NeuroSchedule.

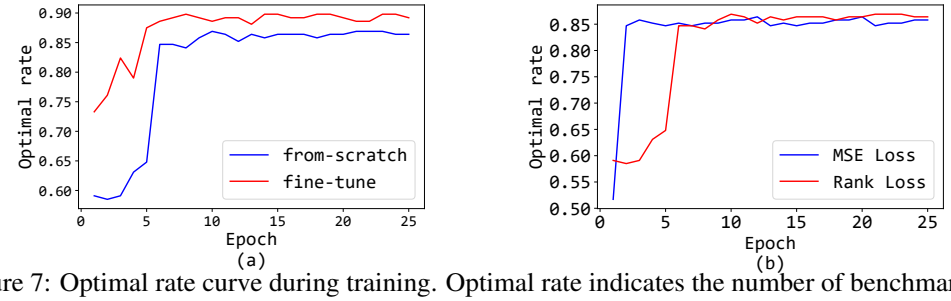

Figure 7: Optimal rate curve during training. Optimal rate indicates the number of benchmarks in the synthesized suite with optimal solutions obtained by NeuroSchedule. (a) Fine-tuning method compared against training from scratch. (b) Training with rank loss function compared against training with MSE loss function.

Nevertheless, NeuroSchedule is still fast and the difference in runtime between NeuroSchedule and entropy-directed algorithm could be ignored.

6.3 Pre-training and Fine-tuning

To answer **Q4**, we synthesize a small dataset that consists of 1000 CDFGs. Details of the small dataset are presented in supplementary materials. Based on the synthesized small dataset, NeuroSchedule is trained in two different ways: from scratch and fined-tuned from the pre-training model. The synthesized benchmark suite in Section 6.1 is adopted to evaluate the two models trained in different ways. Besides, the optimal rate is selected as the metric, which indicates the number of benchmarks in the synthesized suite with optimal solutions obtained by NeuroSchedule. Figure 7 depicts the optimal rate curve during training. As shown in the figure, NeuroSchedule fine-tuned from the pre-training model achieves 3% improvement in the optimal rate compared with that trained from scratch. Moreover, NeuroSchedule fine-tuned from the pre-training model achieves a better optimal rate while costing reduced training efforts compared with that trained from scratch.

6.4 Training Settings

To answer **Q5**, NeuroSchedule is trained with MSE loss and Rank loss [21] on the synthesized small dataset described in Section 6.3. The synthesized benchmark suite in Section 6.1 is adopted to evaluate the two models trained with different loss functions. Besides, the optimal rate is selected as the metric. Figure 7 depicts the optimal curves during training. As shown in the figure, rank loss behaves slightly better than MSE loss, which indicates that training a model for predicting the absolute value requires more effort than training a model for predicting the rank. Therefore, the rank loss is chosen as the default training objective function.

7 Conclusion

This paper presents NeuroSchedule, a novel and effective GNN-based scheduling method for HLS. NeuroSchedule learns to predict operation priorities using GNN models. The predicted priorities are adopted in list scheduling process. Besides, to enhance NeuroSchedule's scalability for various scheduling problems with different settings, pre-training methods are adopted. Experimental results

indicate that NeuroSchedule achieves significantly enhanced solutions compared with the state-of-the-art method. Moreover, NeuroSchedule obtains near-optimal solutions while achieving more than **50,000**× speedup compared with the ILP-based algorithm. Future work includes elaborations on the training details for better tuning, supporting operation chaining, and testing of NeuroSchedule on larger and more complicated benchmarks.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See Section 6 and Section 7.
   (c) Did you discuss any potential negative societal impacts of your work? [N/A]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [N/A]
   (b) Did you include complete proofs of all theoretical results? [N/A]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [No] Our NeuroSchedule will be open-sourced once the paper is accepted.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section 4 and the supplementary materials.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [No]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes]
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] We put the large CDFG dataset into our supplementary materials.
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes] The benchmarks used in our paper are open-sourced, and we cite them in our paper.
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

A Supplementary Materials

A.1 Traditional List Scheduling Algorithm

Algorithm 2 Traditional list scheduling algorithm.

Input: Priority function $\mathcal{F}$, CDFG $G = (V, E)$, functional unit set U, and delay array d
Output: Generated schedule S'

1: $V_F \leftarrow \phi$, $V_R \leftarrow \phi$, $V_U \leftarrow V$, $S' \leftarrow \phi$, $Time \leftarrow 0$
2: **for** v_i in V **do**
3: **if** $v_i.inDegree() = 0$ **then**
4: $V_R \leftarrow V_R \cup v_i$, $V_U \leftarrow V_U \setminus v_i$
5: **while** $|V_F| < |V|$ **do**
6: **for** u_j in U **do**
7: $M \leftarrow MAX_FLOAT$, $v_{chosen} \leftarrow \phi$
8: **for** v_i in V_R **do**
9: **if** $\mathcal{F}(v_i) < M$ **and** $v_i.canUse(u_j)$ **then**
10: $M \leftarrow \mathcal{F}(v_i)$, $v_{chosen} \leftarrow v_i$
11: **if** $v_{chosen} = \phi$ **or** $u_j.unavailable(Time)$ **then**
12: **continue**
13: $S'.insert(v_{chosen}, u_j, Time)$
14: $u_j.setUnavailable(Time, Time + d_{u_j} - 1)$
15: $V_R \leftarrow V_R \setminus v_{chosen}$, $V_F \leftarrow V_F \cup v_{chosen}$
16: **for** v_i in V_R **do**
17: **if** $(v_{chosen}, v_i) \in E$ **then**
18: $E \leftarrow E \setminus (v_{chosen}, v_i)$
19: **if** $v_i \in V_U$ **and** $v_i.inDegree() = 0$ **then**
20: $V_R \leftarrow V_R \cup v_i$, $V_U \leftarrow V_U \setminus v_i$
21: $Time \leftarrow Time + 1$

Algorithm 2 gives an overview of the traditional list scheduling algorithm. Our proposed NeuroSchedule method as shown in Algorithm 1 derives from Algorithm 2, while taking our trained neural network as the priority function. The loop (line 5) runs until each node in the CDFG is successfully scheduled. In each cycle, for every available functional unit (line 6), the algorithm schedules the operation v_{chosen} with the highest priority to the functional unit (line 13). Note that only operations of the corresponding type of the current functional unit can be chosen (line 9). After the chosen operation v_{chosen} is scheduled, all the out edges (v_{chosen}, v_i) of v_{chosen} are deleted (line 18). If the in-degree of v_i equals 0, v_i is added into the ready set V_R (line 20). Finally, the scheduling solution is obtained in S'.

In the traditional list scheduling algorithm, the most widely-used priority function is:

$$\mathcal{F}_t(i) = ALAP(v_i) - ASAP(v_i) \tag{6}$$

where $ASAP$ and $ALAP$ are defined as in Section 3. The priority function $\mathcal{F}_t$ describes the flexibility of each node in the CDFG. This priority function follows a simple but effective rule: nodes with higher flexibility are scheduled prior to nodes with lower flexibility. Recently, the force-directed priority function [12] and the entropy-directed priority function [13] are designed for better scheduling solutions. In the proposed NeuroSchedule method, our GNN-based priority function shows its superiority to other methods.

A.2 Dataset Preparation

It is necessary to acquire sufficient data for training a GNN model to predict the operations' priorities. We propose a CDFG generation algorithm, which generates CDFGs with a balanced structure and high diversity. Algorithm 3 presents the CDFG generation algorithm, where T denotes the number of operations in the generated CDFG, M denotes the minimum number of operations in a layer, N denotes the maximum number of operations in a layer, I denotes the rate that inter-layer operations are connected, U denotes the rate that an operation is not connected to a predecessor, and $G = (V, E)$ denotes the generated CDFG. As shown in the algorithm, operations in the generated CDFG are

arranged into several layers, and operations in the current layer are randomly connected to operations in previous layers.

Algorithm 3 CDFG generation algorithm.

Input: T, M, N, I, U
Output: Generated CDFG $G = (V, E)$

```
L_1 ← φ, L_2 ← φ, L_3 ← φ, V ← φ, E ← φ
while T > 0 do
    C ← random.randint(M, N)
    T ← T − C
    repeat
        C ← C − 1
        O ← newOperation()
        O.optype ← randomOpType()
        V ← V ∪ O
        L_3 ← L_3 ∪ O
        if random.random() > U then
            if random.random() < I then
                O' ← selectRandomElement(L_1)
            else
                O' ← selectRandomElement(L_2)
            E ← E ∪ (O, O')
    until C < 0
    L_1 ← L_1 ∪ L_2
    L_2 ← L_3
    L_3 ← φ
return (V, E)
```

A.3 Dataset Details

Two datasets are synthesized for training and evaluating the proposed model. Details of the synthesized datasets are presented as follows.

First, we synthesize a large dataset including 50000 CDFGs to train our model. The CDFGs are randomly generated using the algorithm shown in Algorithm 3, and the labels are generated using the ILP methods as introduced in Section 4. The numbers of functional units are randomly generated according to the size of CDFG, using the following function:

$$N_{u_i} = randInt(1, \max(1, \left\lfloor \frac{n_{CDFG}}{10} \right\rfloor) \tag{7}$$

Second, a small dataset including 1000 CDFGs are built to evaluate our training settings in Section 5.2. In the small dataset, the number of each functional unit is fixed to 1.

For better scalability on real applications, the dataset is extended to give more instructive information to our GNN model. The node features for each node v_i are a 11-dimensional vector F, and the details are given as follows:

- 0-1 : Operation's type (one-hot);
- 2 : Number of operation's cycles;
- 3 : The scheduling result using ASAP method (normalized);
- 4 : The scheduling result using ALAP method (normalized);
- 5 : $ASAP(v_i)$ as introduced in Section 3;
- 6 : $ALAP(v_i)$ as introduced in Section 3;
- 7 : The scheduling result of traditional list scheduling algorithm using $ALAP - ASAP$ as the priority function;

8 : $\max_{v_i \in V} ASAP(v_i)$;

9 : The maximum number of cycles obtained by traditional list scheduling algorithm;

10 : The number of corresponding functional units u_{v_i}.

Note that features $F[3,4]$ are different from $F[5,6]$, because $F[3,4]$ are the scheduling results using the idea of ASAP and ALAP, while considering the resource constraints. All the node features can be obtained efficiently by the traditional list scheduling algorithm using $ALAP - ASAP$ as the priority function.

A.4 Model details

In our network model, we use a 5-layer GIN [14] to generate the learned operation embeddings. The dimension of each GIN layer is 64. The learned operation embeddings are fed into a $(64, 64)$ dense layer, and then into a $(64, 1)$ dense layer. The activation function of each layer in the model is ReLU. There is a dropout layer between the 5-layer GIN model and the fully connected layers, while the dropout value is set to be 0.5.

A.5 Experiment Configuration

In our training process, we train our model in 2 stages, pre-training and fine-tuning. More specifically, we train our GNN model in the following way:

Stage 1 : **Pre-training:** We use our generated large dataset including 50000 CDFGs to train our model. The dataset is divided into the training set consisting of 49000 CDFGs, and the evaluation set consisting of 1000 CDFGs. The learning rate is set to be 0.0002 initially, which decays by $lr = 0.9 \times lr$ for each 10 epochs. We train the model for 2500 epochs.

Stage 2 : **Fine-tuning:** We use our generated small dataset including 1000 CDFGs to fine-tune our model. The learning rate is set to be 0.0002 initially, which decays by $lr = 0.9 \times lr$ for each 10 epochs. We train the model for 25 epochs.