

A BENCHMARK ON DIRECTED GRAPH REPRESENTATION LEARNING IN HARDWARE DESIGNS

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ABSTRACT

To keep pace with the rapid advancements in design complexity within modern computing systems, directed graph representation learning (DGRL) has become crucial, particularly for encoding circuit netlists, computational graphs, and developing surrogate models for hardware performance prediction. However, DGRL remains relatively unexplored, especially in the hardware domain, mainly due to the lack of comprehensive and user-friendly benchmarks. This study presents a novel benchmark comprising five hardware design datasets and 13 prediction tasks spanning various levels of circuit abstraction. We evaluate 21 DGRL models, employing diverse graph neural networks and graph transformers (GTs) as backbones, enhanced by positional encodings (PEs) tailored for directed graphs. Our results highlight that bidirected (BI) message passing neural networks (MPNNs) and robust PEs significantly enhance model performance. Notably, the top-performing models include PE-enhanced GTs interleaved with BI-MPNN layers and BI-Graph Isomorphism Network, both surpassing baselines across the 13 tasks. Additionally, our investigation into out-of-distribution (OOD) performance emphasizes the urgent need to improve OOD generalization in DGRL models. This benchmark, implemented with a modular codebase, streamlines the evaluation of DGRL models for both hardware and ML practitioners.¹

1 INTRODUCTION

Directed graphs, where edges encode directional information, are widely utilized as data models in various applications, including email communication Kossinets et al. (2008); Khrabrov & Cybenko (2010), financial transactions Gale & Kariv (2007); Chinazzi & Fagiolo (2015); Tiwari et al. (2021), and supply chains Surana et al. (2005); Kaur et al. (2006); Wagner & Neshat (2010). Notably, hardware designs can be represented as directed graphs, such as circuit netlists Hachtel & Somenzi (2005); Vladimirescu (1994), control and data flow graphs Cummins et al. (2021); Wu et al. (2022b); Bai et al. (2023); Ye et al. (2024), or computational graphs Zhang et al. (2021a); Phothilimthana et al. (2023), often exhibiting unique properties. These graph structures reflect restricted connection patterns among circuit components or program operation units, with directed edges encapsulating long-range directional and logical dependencies.

Recently, employing machine learning (ML) to assess the properties of hardware designs via their directed graph representations has attracted significant attention Wu & Xie (2022); Bai et al. (2023); Dong et al. (2023); Li et al. (2020c); Ma et al. (2019b); Bücher et al. (2022); He et al. (2021); Guo et al. (2022); Phothilimthana et al. (2023). Traditional simulation-based methods often require considerable time (hours or days) to achieve the desired accuracy in assessing design quality Zhao et al. (2017); Dai et al. (2018); Wu et al. (2021a; 2022b), substantially slowing down the hardware development cycle due to repeated optimization-evaluation iterations. In contrast, ML models can serve as faster and more cost-effective surrogates for simulators, offering a balanced alternative between simulation costs and prediction accuracy Mirhoseini et al. (2021); Al-Hyari et al. (2021); Wu et al. (2021a); Chen et al. (2018); Jia et al. (2020); Cakir & Malik (2018); Dudziak et al. (2020); Cao et al. (2022); Liu et al. (2021); Wang et al. (2020); Wu et al. (2023). Such an approach is promising to expedite hardware evaluation, especially given the rapid growth of design complexity in modern electronics and computing systems Society.

¹Document (PDF version) and code for the toolbox are provided in supplementary materials.

Despite the promising use cases, developing ML models for reliable predictions on directed graphs, particularly within hardware design loops, is still in its early stages, largely due to the lack of comprehensive and user-friendly benchmarks. Existing studies in the ML community have primarily focused on undirected graphs, utilizing Graph Neural Networks (GNNs) Kipf & Welling (2016); Xu et al. (2019); Veličković et al. (2018) or Graph Transformers (GTs) Rampásek et al. (2022); Kreuzer et al. (2021); Ying et al. (2021); Min et al. (2022). Among the limited studies on directed graph representation learning (DGRL) Zhang et al. (2021b); Tong et al. (2020b;a); Geisler et al. (2023), most have only evaluated their models for node/link-level predictions on single graphs in domains such as web networks, or financial networks He et al. (2024). These domains exhibit very different connection patterns compared to those in hardware design. To the best of our knowledge, CODE2 in the Open Graph Benchmark (OGB) Hu et al. (2020) is the only commonly used benchmark that may share some similarities with hardware data. However, the graphs in CODE2 are IRs of Python programs, which may not fully reflect the properties of data in hardware design loops.

Numerous DGRL models for hardware design tasks have been developed by domain experts. While promising, hardware experts tend to incorporate domain-specific insights with off-the-shelf GNNs (e.g., developing hierarchical GNNs to mimic circuit modules Wu et al. (2022b); Dong et al. (2023) or encoding circuit fan-in and fan-out in node features Ren et al. (2020); Alrahis et al. (2021b); Vasudevan et al. (2021)), with limited common design principles investigated in model development. In contrast, state-of-the-art (SOTA) DGRL techniques proposed by the ML community lack thorough investigation in these tasks. These techniques potentially offer a more general and effective manner of capturing data patterns that might be overlooked by domain experts.

Present Benchmark. This work addresses the aforementioned gaps by establishing a new benchmark consisting of representative hardware design tasks and extensively evaluating various DGRL techniques for these tasks. On one hand, the evaluation results facilitate the identification of commonly useful principles for DGRL in hardware design. On the other hand, the ML community can leverage this benchmark to further advance DGRL techniques.

Specifically, our benchmark collects five hardware design datasets encompassing a total of 13 prediction tasks. The data spans different levels of circuit abstraction, with graph sizes reaching up to 400+ nodes per graph across 10k+ graphs for graph-level tasks, and up to 50k+ nodes per graph for node-level tasks (see Fig. 1 and Table. 1). We also evaluate 21 DGRL models based on 8 GNN/GT backbones, combined with different message passing directions and various enhancements using positional encodings (PEs) for directed graphs Geisler et al. (2023). PEs are vectorized representations of node positions in graphs and have been shown to improve the expressive power of GT/GNNs for undirected graphs Wang et al. (2022a); Huang et al. (2024); Lim et al. (2022); Rampásek et al. (2022). PEs for directed graphs are still under-explored Geisler et al. (2023), but we believe they could be beneficial for hardware design tasks that involve long-range and logical dependencies.

Our extensive evaluations provide significant insights into DGRL for hardware design tasks. Firstly, bidirected (BI) message passing neural networks (MPNNs) can substantially improve performance for both pure GNN encoders and GT encoders that incorporate MPNN layers, such as GPS Rampásek et al. (2022). Secondly, PEs, only when used stably Wang et al. (2022a); Huang et al. (2024), can broadly enhance the performance of both GTs and GNNs. This observation contrasts with findings from undirected graph studies, particularly in molecule property prediction tasks, where even unstable uses of PEs may improve model performance Dwivedi et al. (2023); Kreuzer et al. (2021); Lim et al. (2022); Rampásek et al. (2022). Thirdly, GTs with MPNN layers typically outperform pure GNNs on small graphs but encounter scalability issues when applied to larger graphs.

With these insights, we identify two top-performing models: GTs with BI-MPNN layers (effective for small graphs in the HLS and AMP datasets) and the BI-Graph Isomorphism Network (GIN) Xu et al. (2019), both enhanced by stable PEs. These models outperform all baselines originally designed by hardware experts for corresponding tasks, across all 13 tasks. Notably, this work is the first to consider GTs with BI-MPNN layers and using stable PEs in DGRL, so the above two models have novel architectures essentially derived from our benchmarking effort.

Furthermore, recognizing that hardware design often encounters out-of-distribution (OOD) data in production (e.g., from synthetic to real-world Wu et al. (2022b), before and after technology mapping Wu et al. (2023), inference on different RISC-V CPUs He et al. (2021)), for each dataset we evaluate the methods data with distribution shift to simulate potential OOD challenges. We observe

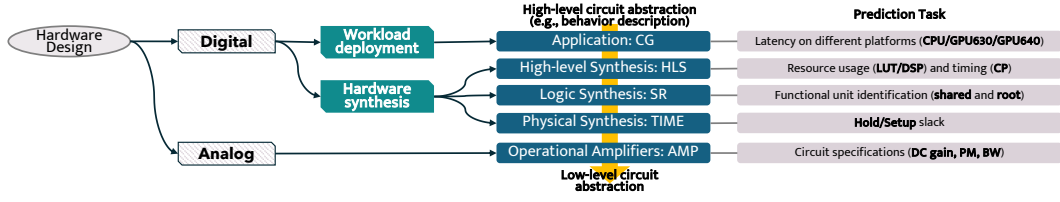


Figure 1: Coverage of Datasets/Tasks.

	High-level Synthesis (HLS) Wu et al. (2022b)	Symbolic Reasoning (SR) Wu et al. (2023)	Pre-routing Timing Prediction (Time) Guo et al. (2022)	Computational Graph (CG) Zhang et al. (2021a)	Operational Amplifiers (AMP) Dong et al. (2023)
Type	digital	digital	digital	digital	analog
Level	graph	node	node	graph	graph
Target	regression	classification	regression	regression	regression
Task	LUT, DSP, CP	node shared by MAJ and XOR, root node of an adder	hold slack, setup slack	CPU/GPU630/GPU640	gain, PM, BW
Evaluation Metric	mse, r2	accuracy, f1 recall, precision	mse, r2	rmse, acc5, acc10	mse, rmse
In-Distribution	CDFG	24-bit	graph structure	network structure	stage3
Out-of-Distribution	DFG	32, 36, 48-bit	graph structure	network structure	stage2
# Training Graph	16570 - 16570	1 - 1	7 - 7	5* - 10000	7223-7223
#Train Nodes	average 95 max 474	4440 4440	29839 58676	218 430	9 16
# Train Edges	average 123 max 636	10348 10348	41268 83225	240 487	15 36

Table 1: Statistics of selected datasets. In row ‘# Training graph’, we report ‘# Graph Structures - # Samples’. *: in CG, there are only five unique CNN designs, yet the structure of graphs within each design may vary slightly.

that while ML models perform reasonably well on tasks (8 of 13) with diverse graph structures in the training dataset, they generally suffer from OOD generalization issues on the remaining tasks. This finding highlights the urgent need for future research to focus on improving the OOD generalization capabilities of DGRL models.

Lastly, our benchmark is implemented with a modular and user-friendly codebase, allowing hardware practitioners to evaluate all 21 DGRL models for their tasks with data in a PyG-compatible format Fey & Lenssen (2019), and allowing ML researchers to advance DGRL methods using the collected hardware design tasks.

2 RELATED WORK

Graph Representation Learning as Powerful Surrogate Models. ML-based surrogate models have been widely adopted in scientific fields Olivier et al. (2021); Zuo et al. (2021) and recently extended in hardware design. While graph-learning-based surrogate models for hardware design have already demonstrated effectiveness Wang et al. (2022b); Ustun et al. (2020); Wu et al. (2022b; 2021a); Bai et al. (2023); Ren et al. (2020); Zhang et al. (2019a); Li et al. (2020c); Ma et al. (2019b); Vasudevan et al. (2021); Bücher et al. (2022); Alrahis et al. (2021b); Lu et al. (2023); Qin et al. (2024); Sohrabizadeh et al. (2023; 2022), several aspects warrant further investigation. First, existing studies often rely on task-specific heuristics to encode circuit structural information Ma et al. (2019b); Ren et al. (2020); Alrahis et al. (2021b); Bücher et al. (2022); Vasudevan et al. (2021); Mirhoseini et al. (2021), hindering the migration of model-design insights from one task to an even closely related task. Second, the majority of these studies conduct message passing of GNNs along edge directions, with few considering BI implementation He et al. (2021); Guo et al. (2022), and there is an absence of a comparative analysis of different DGRL approaches. Third, the designed models are often trained and tested within similar data distributions Alrahis et al. (2021b); Zhao & Shamsi (2022); He et al. (2021), lacking systematic OOD evaluation for new or more complicated designs. Hence, it is imperative to establish a comprehensive benchmark to compare different DGRL approaches for hardware design tasks.

Methods for DGRL. NN architectures for DGRL can be classified into three types: spatial GNNs, spectral GNNs, and transformers. Spatial GNNs use graph topology as inductive bias, some employ bidirectional message passing for regular directed graphs Jaume et al. (2019); Wen et al. (2020); Kollias et al. (2022); Rossi et al. (2024), others use asynchronous message passing exclusively designed for directed acyclic graphs (DAGs) Zhang et al. (2019b); Dong et al. (2022); Thost & Chen (2020).

Spectral GNNs generalize the ideas of Fourier transform and corresponding spectral convolution from undirected to directed graphs Furutani et al. (2020); He et al. (2022); Fiorini et al. (2023); Zhang et al. (2021b); Singh et al. (2016); Ma et al. (2019a); Monti et al. (2018); Tong et al. (2020b); Koke & Cremers (2023); Transformers with attention mechanism reply on designing direction-aware PEs to capture directed graph topology. This benchmark is the first to consider combining transformers with MPNN layers for DGRL, extending the ideas in Rampásek et al. (2022). Regarding the choices of PEs, most studies are on undirected graphs Wang et al. (2022a); Huang et al. (2024); Lim et al. (2022); Dwivedi et al. (2022a). For directed graphs, the potential PEs are Laplacian eigenvectors of the undirected graphs by symmetrizing the original directed ones Dwivedi et al. (2023), singular vectors of adjacency matrices Hussain et al. (2022) and the eigenvectors of Magnetic Laplacians Shubin (1994); Fanuel et al. (2017; 2018); Geisler et al. (2023). No previous investigate benefit for DGRL from stably incorporating PE Wang et al. (2022a); Huang et al. (2024), and we are the first to consider stable PEs for DGRL.

Existing Relevant Benchmarks. Dwivedi et al. (2022b) benchmark long-range reasoning of GNNs on undirected graphs; PyGSD He et al. (2024) benchmarks signed and directed graphs, while focusing on social or financial networks. We also compare all the methods for directed unsigned graphs in PyGSD and notice that the SOTA spectral method therein - MagNet Zhang et al. (2021b) still works well on node-level tasks on a single graph (SR), which shares some similar insights. The hardware community has released graph-structured datasets from various development stages to assist surrogate model development, including but not limited to NN workload performance Zhang et al. (2021a); Phothilimthana et al. (2023), CPU throughput Chen et al. (2019); Sýkora et al. (2022); Mendis et al. (2019), resource and timing in HLS Wu et al. (2022b); Bai et al. (2023), design quality in logic synthesis Chowdhury et al. (2021), design rule checking in physical synthesis Guo et al. (2022); Chai et al. (2023); Xun et al. (2024); Chhabria et al. (2024), and hardware security Yu et al. (2021). In addition to datasets, ProGraML Cummins et al. (2021) introduces a graph-based representation of programs derived from compiler IRs (e.g., LLVM/XLA IRs) for program synthesis and compiler optimization. Very recently, Google launched TPUgraph for predicting the runtime of ML models based on their computational graphs on TPUs Phothilimthana et al. (2023). Our CG dataset includes computational graphs of ML models, specifically on edge devices.

3 DATASETS AND TASKS

This section introduces the five datasets with thirteen tasks used in this benchmark. The datasets cover both digital and analog hardware, considering different circuit abstraction levels, as illustrated in Fig. 1. Table 1 displays the statistics of each dataset. Next, we briefly introduce the five datasets, with details provided in Appendix. D. Although these datasets are generated by existing studies, we offer modular pre-processing interfaces to make them compatible with PyTorch Geometric and user-friendly for integration with DGRL methods.

High-Level Synthesis (HLS) Wu et al. (2022b): The HLS dataset collects IR graphs of C/C++ code after front-end compilation Alfred et al. (2007), and provides post-implementation performance metrics on FPGA devices as labels for each graph, which are obtained after hours of synthesis with Vitis vit and implementation with Vivado viv. The labels to predict include resource usage, (i.e., look-up table (LUT) and digital signal processor (DSP)), and the critical path timing (CP). See Appendix. D.1 for graph input details.

Significance: The HLS dataset is crucial for testing NNs’ ability to accurately predict post-implementation metrics to accelerate design evaluation in the stage of HLS.

OOD Evaluation: For training and ID testing, we use control data flow graphs (CDFG) that integrate control conditions with data dependencies, derived from general C/C++ code; As to OOD cases, we use data flow graphs (DFG) derived from basic blocks, leading to distribution shifts.

Symbolic Reasoning (SR) Wu et al. (2023): The SR dataset collects bit-blasted Boolean networks (BNs) (unstructured gate-level netlists), with node labels annotating high-level abstractions on local graph structures, e.g., XOR functions, majority (MAJ) functions, and adders, generated by the logic synthesis tool ABC Brayton & Mishchenko (2010). Each graph supports two tasks: root nodes of adders, and nodes shared by XOR and MAJ functions. See Appendix. D.2 for detailed input encoding and label explanation.

Significance: Reasoning high-level abstractions from BNs has wide applications in improving functional verification efficiency Ciesielski et al. (2019) and malicious logic identification Mahzoon et al. (2019). GNN surrogate models are anticipated to replace the conventional structural hashing and functional propagation Li et al. (2013); Subramanyan et al. (2013) and boost the scalability with significant speedup. For graph ML, due to significant variation in the size of gate-level netlists under different bit widths, SR is an ideal real-world application to evaluate whether GNN designs can maintain performance amidst the shifts in graph scale.

OOD Evaluation: We use a 24-bit graph (4440 nodes) for training, and 32, 36, 48-bit graphs (up to 18096 nodes) for ID testing, derived from carry-save-array multipliers before technology mapping. OOD testing data are multipliers after ASAP 7nm technology mapping Xu et al. (2017) with the same bits.

Pre-routing Timing Prediction (TIME) Guo et al. (2022): The TIME dataset collects real-world circuits with OpenROAD ope (b) on SkyWater 130nm technology sky. The goal is to predict slack values at timing endpoints for each circuit design by using pre-routing information. Two tasks are considered: hold slack and setup slack. Details are provided in Appendix. D.3.

Significance: In physical synthesis, timing-driven placement demands accurate timing information, which is only available after routing. Repetitive routing and static timing analysis provide accurate timing but are prohibitively expensive. ML models that precisely learn routing behaviors and timing computation flows are highly expected to improve the efficiency of placement and routing.

OOD Evaluation: We divide ID-OOD based on the difference in graph structures (e.g. ‘blabla’ and ‘xtea’ are different circuit designs, allocated into ID or OOD groups). See details in Appendix. D.3.1.

Computational Graph (CG) Zhang et al. (2021a): The CG dataset consists of computational graphs of convolutional neural networks (CNNs) with inference latency on edge devices (i.e., Cortex A76 CPU, Adreno 630 GPU, Adreno 640 GPU) as labels. The CNNs have different operator types or configurations, either manually designed or found by neural architecture search (NAS). Details are in Appendix. D.4.

Significance: Accurately measuring the inference latency of DNNs is essential for high-performance deployment on hardware platforms or efficient NAS Ren et al. (2021); Shi et al. (2022), which however is often costly. ML-based predictors offer the potential for design exploration and scaling up to large-scale hardware platforms.

OOD Evaluation: We split ID-OOD with different graph structures. (e.g. ‘DenseNets’ and ‘ResNets’ are CNNs with different structures, allocated into different groups). See Appendix. D.4.1 for details.

Operational Amplifiers (AMP) Dong et al. (2023): AMP dataset contains 10,000 distinct 2- or 3-stage operational amplifiers (Op-Amps). Circuit specifications (i.e. DC gain, phase margin (PM), and bandwidth (BW)) as labels are extracted after simulation with Cadence Spectre spe. Details are in Appendix. D.5.

Significance: Analog circuit design is less automated and requires more manual effort compared to its digital counterpart. Mainstream approaches such as SPICE-based circuit synthesis and simulation Vladimirescu (1994), are computationally expensive and time-consuming. If ML algorithms can approximate the functional behavior and provide accurate estimates of circuit specifications, they may significantly reduce design time by minimizing reliance on circuit simulation Afacan et al. (2021).

OOD Evaluation: For training and ID testing, we use 3-stage Op-Amps, which have three single-stage Op-Amps in the main feed-forward path). For OOD evaluation, we use 2-stage Op-Amps.

Extensions Although the datasets cover different levels of circuit abstraction, there are additional tasks in hardware design worth exploration with DGRL surrogates, as reviewed in Section 2. Our modular benchmark framework allows for easy extension to accommodate new datasets.

4 BENCHMARK DESIGN

4.1 DESIGN SPACE FOR DIRECTED GRAPH REPRESENTATION LEARNING

In this section, we introduce the DGRL methods evaluated in this benchmark. Our evaluation focuses on four design modules involving GNN backbones, message passing directions, transformer selection, and PE incorporation, illustrated in Fig. 2. Different GNN backbones and transformer adoptions cover

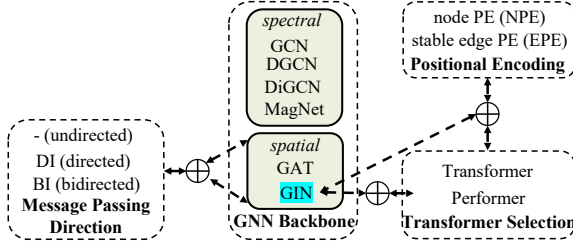


Figure 2: The benchmark considers 21 combinations of message passing direction, GNN backbone, transformer selection and PE incorporation, covers 10 existing SOTA methods from graph ML community and discovers 2 novel top-performing models (see Table. 2).

Method	type	layer-wise complexity
GCN Kipf & Welling (2016)	spectral	$O(E)$
MagNet Zhang et al. (2021b)	spectral	$O(E)$
DGCN Tong et al. (2020b)	spectral	$O(E)$
DiGCN Tong et al. (2020a)	spectral	$O(E)$
GAT Veličković et al. (2018)	spatial	$O(E)$
GIN(E) Xu et al. (2019)	spatial	$O(E)$
EDGNN Jaume et al. (2019)	spatial	$O(E)$
GPS-T Rampáček et al. (2022)	spatial+transformer	$O(V ^2 + E)$
GPS-P Choromanski et al. (2020)	spatial+transformer	$O(V + E)$
TmD Geisler et al. (2023)	transformer	$O(V ^2)$
BI-GIN(E)+EPE(new)	spatial	$O(E)$
BI-GPS-T+EPE(new)	spatial+transformer	$O(V ^2 + E)$

Table 2: Existing methods and two top-performing methods highlighted at bottom.

10 methods in total with references in Tab. 2. We also consider their combinations with different message-passing directions and various ways to use PEs, which overall gives 21 DGRL methods.

For GNNs, we consider 4 spectral methods, namely GCN Kipf & Welling (2016), DGCN Tong et al. (2020b), DiGCN Tong et al. (2020a) and MagNet Zhang et al. (2021b), where the latter three are *SOTA spectral GNNs* specifically designed for DGRL He et al. (2024); For spatial GNNs, we take GIN Xu et al. (2019) and Graph Attention Network (GAT) Veličković et al. (2018), which are the most commonly used MPNN backbones for undirected graphs. We evaluate the combination of GCN, GIN and GAT with three different message-passing directions: a) ‘undirected’ (-) treats directed graphs as undirected, using the same NN parameters to perform message-passing along both forward and reverse edge directions; b) ‘directed’ (DI) only passes messages exclusively along the forward edge directions; c) ‘bidirected’ (BI) performs message passing in both forward and reverse directions with distinct parameters for either direction. The other GNNs (DGCN, DiGCN and MagNet) adopt spectral convolution that inherently considers edge directions. The combination of ‘BI’ with spatial GNN layers gives *the state-of-the-art spatial GNNs* for DGRL, i.e., EDGNN Jaume et al. (2019).

For GTs, we adopt the eigenvectors of the graph Magnetic Laplacian (MagLAP) matrix as the PEs of nodes Furutani et al. (2020); Shubin (1994), as they are directional-aware. The MagLap matrix L_q is a complex Hermitian matrix with parameter $q \in [0, 1)$ named potential, which is treated as a hyper-parameter in our experiments. Note that when $q = 0$, MagLap degenerates to the symmetric Laplacian matrix L_0 as a special case. See Appendix B for a brief review of MagLap. The GT with the MagLap PEs attached to node features gives *the SOTA GT model* for DGRL, named TmD for brevity, proposed in Geisler et al. (2023). GPS Rampáček et al. (2022) is a GT model with MPNN layers Hamilton et al. (2017); Gilmer et al. (2017) interleaving with transformer layers Vaswani et al. (2017), originally proposed for undirected graphs. We extend GPS to directed graphs by using MagLap PEs for transformer layers and DI/BI message passing in its MPNN layers. Hence, GPS is also an extension of TmD by incorporating MPNN layers. As transformers may not scale well on large graphs, we evaluate vanilla transformer layers and their lower-rank approximation Performer Kreuzer et al. (2021) for efficient computation, named as GPS-T and GPS-P, respectively.

4.2 STABLE DIRECTION-AWARE POSITIONAL ENCODINGS

Recent studies on undirected graphs have demonstrated that models by naively attaching PEs to node features may suffer from an issue of instability because small changes in the graph structure may cause big changes in PEs Wang et al. (2022a); Huang et al. (2024); Lim et al. (2022). We name this way of using PEs as node-PE (NPE). The instability provably leads to undesired OOD generalization Huang et al. (2024). We think this is also true for directed graphs and indeed observe the subpar model performance with NPE.

$$\begin{aligned} \mathbf{NPE} &= [\text{Re}\{\mathbf{V}_q\}, \text{Im}\{\mathbf{V}_q\}] \\ \mathbf{EPE} &= \rho(\text{Re}\{\mathbf{V}_q \text{diag}(\kappa_1(\lambda)) \mathbf{V}_q^\dagger\}, \dots, \text{Re}\{\mathbf{V}_q \text{diag}(\kappa_m(\lambda)) \mathbf{V}_q^\dagger\}, \\ &\quad \text{Im}\{\mathbf{V}_q \text{diag}(\kappa_1(\lambda)) \mathbf{V}_q^\dagger\}, \dots, \text{Im}\{\mathbf{V}_q \text{diag}(\kappa_m(\lambda)) \mathbf{V}_q^\dagger\}) \end{aligned}$$

Table 3: Functions to obtain PEs. NPE directly concatenates the eigenvectors to node features. In contrast, before concatenating PE to the edge features, EPE employs the permutation equivariant functions $\kappa : \mathbb{R}^d \rightarrow \mathbb{R}^d$ w.r.t. eigenvalue permutations and permutation equivariant function $\rho : \mathbb{R}^{|V| \times |V| \times 2m} \rightarrow \mathbb{R}^{|V| \times |V| \times d}$ to stably process the eigenvectors and eigenvalues, respectively.

Therefore, besides NPE, we also consider a stable way of incorporating PEs for DGRL, namely ‘edge PE’ (EPE), inspired by Wang et al. (2022a). EPE was originally proposed for the undirected graph case. Specifically, we use the smallest d eigenvalues $\lambda_q \in \mathbb{R}^d$ and their corresponding eigenvectors $\mathbf{V}_q \in \mathbb{C}^{|V| \times d}$ from \mathbf{L}_q . Then, we follow the equation in Table 3 to compute $\mathbf{EPE} \in \mathbb{R}^{|V| \times |V| \times d}$. Then, in GTs, $\mathbf{EPE}_{u,v}$ is further added to the attention weight between nodes u and v as a bias term at each attention layer.

We note that PEs can also be used in more than GTs, to improve the expressive power of GNNs Li et al. (2020b); Ying et al. (2021); Lim et al. (2022); Huang et al. (2024). We leverage this idea and enhance the GNN models for directed graphs with PEs. Specifically, for the GNNs NPE will use \mathbf{NPE}_v as extra node features of node v while EPE will use $\mathbf{EPE}_{u,v}$ as extra edge features of edge uv if uv is an edge.

The incorporation with EPE helps discover a novel GT model for directed graphs, i.e., GT with BI-MPNN layers enhanced by EPE, abbreviated as BI-GPS+EPE. We also make the first attempt to combine GNNs with PEs for directed graphs, which yields the model BI-GIN(E)+EPE.

4.3 HYPER-PARAMETER SPACE AND TUNING

For each combination of DGRL method in this benchmark, we perform automatic hyper-parameter tuning with RAY Liaw et al. (2018) adopting Tree-structured Parzen Estimator (TPE) Watanabe (2023), a state-of-the-art bayesian optimization algorithm. The hyper-parameter space involves searching batch size, learning rate, number of backbone layers, dropout rate in MPNN and MLP layers, hidden dimension, and MLP layer configurations. The detailed hyper-parameter space of each model is shown in Appendix. E.2. We auto-tune the hyper-parameters with seed 123 with 100 trial budgets and select the configuration with the best validation performance. Then, the selected configuration is used for model training and testing ten times with seeds 0 – 9 and the average is reported as the final performance.

5 MODULAR TOOLBOX

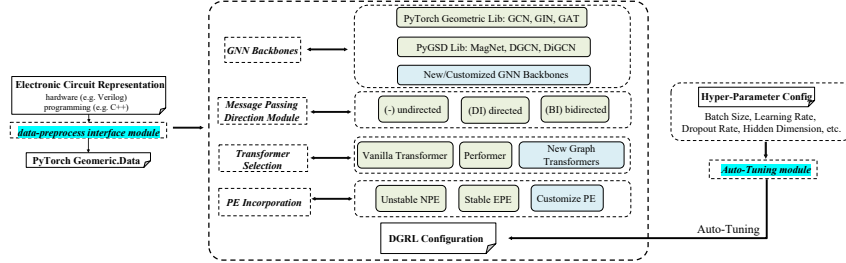


Figure 3: Illustration of the directed graph representation learning (DGRL) toolbox.

We develop a highly modular toolbox involving designing, auto hyper-parameter tuning, and evaluation for DGRL methods. The framework is shown in Fig. 3. The toolbox comes with the 21 DGRL methods, allowing practitioners to evaluate them on any new task with data compatible with PyTorch Geometric (PyG) Fey & Lenssen (2019). This may be used even beyond hardware design applications. Users can also customize new methods. Once the method is configured, auto hyper-parameter tuning can be performed using RAY Liaw et al. (2018). The toolbox also includes the above 5 datasets with 13 tasks that can be used to develop new DGRL models. For details please refer to the official document for this toolbox.

6 EXPERIMENTS

In this section, we first evaluate DGRL methods combining different GNN backbones, message passing directions, transformer selection, and PE incorporation, across all 5 datasets and 13 tasks, using in-distribution (ID) and out-of-distribution (OOD) testing data.

Distribution		In-Distribution (ID)														Out-of-Distribution (OOD)																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
Dataset		HLS					AMP					SR				TIME					CG					HLS					AMP					SR				TIME					CG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
Task		DSP	LUT	CP	gain	PM	BW	share	root	hold	setup	CPU	GPU630	GPU640	DSP	LUT	CP	gain	PM	BW	share	root	hold	setup	CPU	GPU630	GPU640	DSP	LUT	CP	gain	PM	BW	share	root	hold	setup	CPU	GPU630	GPU640																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
Spectral	DGCN	15.0	15.0	15.0	14.0	8.0	15.0	10.0	9.0	15.0	5.5	13.0	15.0	14.0	15.0	15.0	14.0	15.0	14.0	15.0	14.0	15.0	7.5	5.0	15.0	7.0	13.3	11.7	11.2	15.0	14.0	15.0	14.0	3.0	15.0	7.5	5.0	15.0	7.0	13.3	11.7	11.2																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
	DiGCN	12.0	14.0	13.0	12.0	9.0	14.0	8.5	7.8	13.5	15.0	14.0	14.0	14.0	15.0	12.5	15.0	14.0	9.0	4.0	14.0	9.0	5.0	13.5	14.0	13.2	13.3	13.3	12.0	14.0	13.0	12.0	9.0	4.0	14.0	9.0	5.0	13.5	14.0	13.2	13.3																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
	MagNet	7.0	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	7.0	10.5	3.0	12.0	8.0	3.5	8.8	9.0	7.0	4.2	8.2	7.3	7.0	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3	3.3	4.7	7.0	10.5	8.0	11.0	8.0	3.3	3.3	11.0	11.5	3.3

Table 4: Average ranking (\downarrow) of methods across datasets/tasks/metrics on ID and OOD data.

Distribution		In-Distribution (ID)														Out-of-Distribution (OOD)																															
Dataset		HLS					AMP					SR				TIME				CG					HLS					AMP					SR				TIME				CG				
Task		DSP	LUT	CP	gain	PM	BW	share	root	hold	setup	CPU	GPU630	GPU640		DSP	LUT	CP	gain	PM	BW	share	root	hold	setup	CPU	GPU630	GPU640		DSP	LUT	CP	gain	PM	BW	share	root	hold	setup	CPU	GPU630	GPU640					
MagNet		14.5	11.0	14.5	12.0	15.0	12.0	2.3	2.3	13.0	13.0	2.3	1.7	6.7		11.0	11.0	14.5	3.0	16.0	12.0	5.5	10.8	11.0	16.0	5.2	9.5	8.3																			
BI-GIN(E)		9.0	2.0	9.0	6.0	6.0	6.0	4.8	6.8	2.5	2.0	6.0	3.3	6.0		7.5	3.5	6.0	4.0	13.0	5.0	3.0	3.0	2.5	3.5	4.7	5.8	4.8																			
BI-GIN(E)+NPE		5.0	4.0	5.0	5.0	13.0	5.0	3.0	6.8	5.5	5.0	8.3	5.0	5.3		9.0	4.0	3.5	7.0	8.0	7.0	2.8	3.5	5.5	12.5	6.0	4.8	6.0																			
BI-GIN(E)+EPE		5.0	1.0	5.0	9.0	10.0	3.5	4.0	6.8	2.0	1.0	1.0	6.7	1.7		7.0	1.0	2.5	6.0	6.0	4.0	1.5	3.0	1.0	7.5	3.5	5.5	4.7																			
BI-GPS-T (NPE)		4.5	5.5	4.5	2.0	2.0	7.0	--	--	--	--	--	--	--		4.0	7.0	8.0	9.0	2.0	6.5	--	--	--	--	--	--	--																			
BI-GPS-T+EPE		2.5	3.0	2.0	1.0	1.0	4.0	--	--	--	--	--	--	--		1.5	1.5	3.5	5.5	1.0	1.0	--	--	--	--	--	--	--																			

Table 5: Comparison of competitive methods involving NPE and EPE. The ranking (\downarrow) is based on all the 18 methods in Table 4 plus BI-GIN(E)+NPE, BI-GIN(E)+EPE and BI-GPS-T+EPE.

6.1 MAIN RESULTS

The performances of the methods under all evaluation metrics for both in-distribution and out-of-distribution testing across all 13 tasks are reported from Table. 11 to Table. 33 in Appendix. H.1. We summarize the averaged ranking with respect to all evaluation metrics given a task in Table. 4. The details of ranking calculation is in Appendix. G.1. The results tell the following insights:

‘Bidirected’ (BI) message passing in the MPNN layers significantly boosts the models’ performance on three GNN backbones (GCN, GIN, GAT) and one GT backbone (GPS-T): BI-GCN outperforms GCN on 10 out of 13 tasks in both ID and OOD evaluations. Similarly, in ID/OOD evaluations, BI-GIN outperforms GIN in 11/12 out of 13 tasks, BI-GAT outperforms GAT in 11/9 out of 13 tasks and BI-GPS-T outperforms GPS-T in 5/5 out of 6 tasks, respectively.

As to the models, on datasets with small graphs (HLS and AMP), BI-GPS-T consistently delivers excellent results, achieving top-3 performance in 5 out of 6 tasks on both ID and OOD testing data. BI-GIN also demonstrates competitive performance on these datasets. However, for datasets with larger graphs (SR, CG, and TIME), BI-GPS-T encounters a scalability issue. BI-GIN secures top-three performance in 6 out of 7 tasks in both ID and OOD testing data. For the ‘shared’ and ‘root’ tasks from the SR dataset and the ‘CPU’ and ‘GPU630’ tasks from the CG dataset, MagNet Zhang et al. (2021b) performs best in the ID setting. This is likely because training and testing are conducted on the same graph structures for these specific datasets, reducing the need for significant generalization across different graph structures. This scenario aligns well with the spectral filtering approach used by MagNet. These observations match findings from previous studies on directed networks Zhang et al. (2021b); He et al. (2024). However, MagNet’s performance falters in OOD evaluations which ask for the ability to generalize across different graph structures. GPS-P, despite its capability to handle large graphs, delivers only mediocre performance overall. *In conclusion, BI-GPS is well-suited for small (around one hundred nodes) directed graphs. For larger graphs, BI-GIN is efficient and performs well. For tasks where the training and testing data share the same graph structures, one may also attempt to adopt MagNet.*

Comparing PE-enhanced methods: We further investigate the impact of different ways of using PEs. We combine NPE or EPE with the top-performing models from the previous section and evaluate BI-GIN+NPE, BI-GIN+EPE, and BI-GPS+EPE. Note that BI-GPS already utilizes NPE. We have chosen not to consider adding PE to MagNet because MagNet only accepts 1-dimensional edge weights, limiting its ability to leverage EPE. We provide a summary of the performance data from

dataset (baseline's name)	AMP Dong et al. (2023) (CKTGNN)			HLS Wu et al. (2022b) (Hierarchical GNN)			SR Wu et al. (2023) (GAMORA)	CG Zhang et al. (2021a) (nn-meter)			TIME Guo et al. (2022) (Timer-GNN)
task	gain	PM	BW	dsp	lut	cp	shared	cpu (average)			hold
metric	rmse↓	rmse↓	rmse↓	mse↓	mse↓	mse↓	accuracy↑	rmse↓	acc5↑	acc10↑	r2↑
Baseline	0.52	1.15	4.47	3.94	2.45	0.88	0.99	3.20	0.80	0.99	0.97
BI-GIN+EPE	0.51±0.07	1.14±0.00	4.20±0.13	2.13±0.08	1.73±0.10	0.61±0.02	0.99±0.00	2.79±0.14	0.86±0.02	0.99±0.01	0.99±0.00
BI-GPS-T+EPE	0.34±0.08	1.15±0.00	3.79±0.11	2.13±0.15	1.96±0.13	0.60±0.01	--	--	--	--	--

Table 6: Comparison of BI-GIN+EPE and BI-GPS-T+EPE with baselines specific for each dataset. Table 34 to Table 43 in Appendix H.2 and report the average rankings of the methods for each task. All 18 methods in Table 4, along with the 3 new combinations, are included in the ranking. We detail the results of the most competitive methods in Table 5. For BI-GIN, EPE enhances its performance on 10 out of 13 tasks in the in-distribution (ID) testing data and 11 tasks in the out-of-distribution (OOD) testing data. Conversely, NPE only improves the performance of BI-GIN on 7 tasks in the ID testing and 4 tasks in the OOD testing and performs unstable for the rest tasks. Notably, EPE-enhanced BI-GIN surpasses MagNet on the CPU task in the CG dataset. For BI-GPS-T, EPE improves its performance on all 6 tasks in both ID and OOD testing, while NPE does not yield substantial improvements. This observation contrasts with previous work Rampásek et al. (2022) on undirected graphs for molecular property prediction. *In conclusion, we find that incorporating PEs in a stable way as EPE significantly boosts the performance of different models across the selected tasks and datasets.*

6.2 SUMMARY: THE RECIPE FOR DGRL

Through benchmarking various combinations within the design space, we have formulated a design recipe for DGRL methods tailored for encoding hardware data: *The use of 'bidirected' (BI) message passing and stable positional encodings (PE) can significantly enhance model performance. Therefore, we recommend BI-GPS-T+EPE for encoding small graphs and BI-GIN+EPE for large graphs.*

We further compare the two models' performance with the baseline methods proposed by hardware design practitioners specifically for the corresponding tasks in the original papers. Results are shown in Table. 6. The comparison focuses on ID evaluation as for most of the tasks, the original studies did not even report OOD evaluations. We follow the same data split as baseline methods for fair comparison (see the details in Appendix C). BI-GIN+EPE achieves results comparable to, or better than, the baseline methods. BI-GPS+EPE achieves even better performance than BI-GIN+EPE for small graphs. Note that the baseline methods for certain tasks may incorporate domain-specific expert knowledge and additional data processing. For example, CKTGNN Dong et al. (2023) for the AMP dataset modifies the graph structures into DAGs and employs an asynchronized message passing to mimic the signal flow in these amplifiers; 'timer-GNN' Guo et al. (2022) is tailored for the TIME dataset to mimic the transmission rules of clock signals and designs a non-linear delay model (NLDM) along with a novel module 'cell library'. Such domain knowledge may further enhance BI-GPS+EPE and BI-GIN+EPE for these specific tasks, which is left for future research.

Discussion on OOD Evaluation: Despite BI-GPS-T+EPE and BI-GIN+EPE outperforming other methods in OOD testing across all tasks, we cannot yet conclude that these methods are sufficiently effective for practical OOD usage. *In fact, making accurate predictions with OOD data in hardware design remains a significant challenge.* When the graph structures in training sets are sufficiently diverse, such as in datasets with a large number of small graphs (e.g., AMP, HLS) or those with abundant local structures (e.g., SR), BI-GIN+EPE and BI-GPS-T+EPE tend to maintain reasonably good performance on OOD data. However, OOD generalization becomes challenging when the diversity of graph structures in the training set is limited. For instance, in the TIME dataset, which has a limited variety of graph structures for training and OOD testing data with entirely different graph structures, both BI-GIN+EPE and BI-GPS-T+EPE perform worse than timer-GNN Guo et al. (2022), which integrates the knowledge of the physical structure of circuits (as shown in Table 21). We identify ensuring OOD performance, especially when training sets lack sufficiently diversified graph structures, as a key direction for future DGRL research.

7 CONCLUSIONS AND LIMITATIONS

Through benchmarking 21 methods on in-distribution and out-of-distribution test sets across 13 tasks and 5 datasets within the hardware design loop, we find bidirected (BI) message passing neural networks can substantially improve the performance of both Graph Transformer (GT) encoders that incorporate MPNN layers and pure GNN encoders. Positional Encodings (PEs), particularly when

used stably, can broadly enhance the performance of both GTs and GNNs. With these insights, we identify two top-performing models: BI-GPS-T+EPE and BI-GIN+EPE, both of which outperform the baseline models originally proposed for the corresponding tasks.

Limitations: Although the benchmark covers multiple stages in hardware design loop, there are other tasks Mendis et al. (2019); Sýkora et al. (2022); Xun et al. (2024); Chai et al. (2023); Chen et al. (2019); Alrahis et al. (2021b); Zhang et al. (2019a) that could be included in this benchmark as DGRL tasks. Given technological advancements and the diversity of design tools, ensuring OOD performance remains an urgent open problem in hardware design. Future research may involve high-quality data collection Jain et al. (2020); Gupta et al. (2021); Wu et al. (2021b); Whang et al. (2023); Wu et al. (2020) or the development of OOD-aware DGRL methods Liu et al. (2023); Shi et al. (2024); Liu et al. (2024); Liu & Ding (2024).

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A MORE RELATED WORK

In this section, we review the extensive previous studies that use ML-based surrogate models.

ML-based surrogate models have been widely used in hardware system design, such as predicting energy/power consumption, latency, throughput, or reliability on CPUs Lo et al. (2015); Zheng et al. (2016); Mishra et al. (2018); Mendis et al. (2019); Lin et al. (2019); Chen et al. (2019); Sýkora et al. (2022), GPUs Jia et al. (2012); Baldini et al. (2014); O’Neal et al. (2017); Pattnaik et al. (2016); Chen et al. (2018); Li et al. (2020a), tensor processing units (TPUs) Kaufman et al. (2021); Phothilimthana et al. (2023), and data centers Murray et al. (2005); Mahdisoltani et al. (2017); Xu et al. (2018). Similar trends are observed in quickly estimating quality-of-results of circuit designs in EDA flows, spanning high-level synthesis (HLS) Wang et al. (2022b); Zhao et al. (2019); Makrani et al. (2019); Ustun et al. (2020); Lin et al. (2020); Wu et al. (2022b; 2021a); Bai et al. (2023); Ye et al. (2024), logic synthesis Yu et al. (2018); Yu & Zhou (2020); Wu et al. (2022a; 2023); Zhao & Shamsi (2022), physical synthesis Tabrizi et al. (2018); Liang et al. (2020); Chen et al. (2020); Mirhoseini et al. (2021); Guo et al. (2022); Esmailzadeh et al. (2023); Lu et al. (2024; 2020), analog circuit designs Wang et al. (2020); Zhang et al. (2019a); Ren et al. (2020); Shook et al. (2020); Li et al. (2020c); Dong et al. (2023), and design verification Ma et al. (2019b); Hughes et al. (2019); Shibu et al. (2021); Vasudevan et al. (2021); Wu et al. (2024). *As circuits can naturally be represented as directed graphs, the adoption of GNN-based surrogate models is increasingly prominent.* We discuss several examples for each of the aforementioned tasks as follows.

In CPU throughput estimation, Granite Sýkora et al. (2022) adopts a GNN model to predict basic block throughput on CPUs. Basic blocks are represented as graphs to capture the semantic relationships between instructions and registers. A GNN model is then trained to learn expressive embeddings for each basic block, followed by a decoder network to predict the throughput.

In HLS, many studies leverage the IR graphs generated by HLS front-ends. Ustun et al. (2020) employs GNNs to predict the mapping from arithmetic operations in IR graphs to different resources on FPGAs. GNN-DSE Sohrabizadeh et al. (2022) also apply graph neural network to learn resource consumption mappings on HLS codes. Sohrabizadeh et al. (2023) propose Harp, a hierarchical abstract of the HLS graph, Qin et al. (2024) apply pre-trained language models with GNNs to conduct multi-modality prediction on the mapping. IronMan Wu et al. (2021a) exploits GNNs to generate graph embeddings of IR graphs, which serve as state representations in its reinforcement learning (RL-)based search engine to find the Pareto curve between two types of computing resources on FPGAs. The same problem can also be solved by carefully designing a GNN surrogate model as a continuous relaxation of the actual cost model, allowing for a soft solution that can be decoded into the final discrete solution of resource assignments Wang et al. (2022b). In terms of HLS datasets, Wu et al. (2022b) develop an HLS dataset and benchmark GNNs for predicting resource usage and timing, however, they enhance accuracy with domain-specific information and do not explore message passing directions or the benefit from positional encoding. Bai et al. (2023) contribute a new HLS dataset and combine pre-trained language models Wang et al. (2021); Guo et al. (2020) and GNNs to predict the optimization effects of different directives.

In logic synthesis or logic design, LOSTIN Wu et al. (2022a) employs a GNN to encode circuit graphs and an LSTM to encode logic synthesis sequences, where the two embeddings are concatenated to predict logic delay and area. To identify functional units from gate-level netlists, different GNN models can be leveraged to classify sub-circuit functionality Alrahis et al. (2021a), predict the functionality of approximate circuits Bücher et al. (2022), analyze impacts of circuit rewriting on functional operator detection Zhao & Shamsi (2022), and predict boundaries of arithmetic blocks He et al. (2021). Gamora Wu et al. (2023) leverages the message-passing mechanism in GNN computation to imitate structural shape hashing and functional propagation in conventional symbolic reasoning, achieving up to six orders of magnitude speedup compared to the logic synthesis tool ABC in extracting adder trees from multipliers.

In physical synthesis, Mirhoseini et al. (2021) combine GCN with deep RL to place macros (i.e., memory cells), after which standard cells are placed by a force-directed method. The GCN model encodes the topological information of chip netlists to generate graph embeddings as the inputs to the RL agent, as well as to provide proxy rewards to guide the search process. Lu et al. (2020) apply GraphSAGE Hamilton et al. (2017) to circuit netlists to learn node representations

that capture logical affinity. These representations are grouped by a weighted K-means clustering to provide placement guidance, informing the placer about which cells should be placed nearby in actual physical layouts. Guo et al. (2022) develop a hierarchical GNN with BI message passing to estimate post-routing timing behaviors by using circuit placement results.

In hardware design verification, test point insertion is a common technique aimed at enhancing fault coverage, which modifies target hardware designs by inserting extra control points or observation points. Ma et al. (2019b) use GCNs to predict whether a node in hardware designs is easy or hard to observe, based on which new observation points are inserted. To improve branch coverage, Vasudevan et al. (2021) exploit IPA-GNN (Bieber et al. (2020)) to predict the probability of current test parameters covering specific cover points by characterizing RTL semantics and computation flows; new tests targeting uncovered points are generated by maximizing the predicted probability with respect to test parameters through gradient-based search.

In analog circuit design, by using circuit schematics, CktGNN (Dong et al. (2023)) employs a nested GNN to predict analog circuit properties (i.e., gain, BW, PM) and reconstruct circuit topology. By using pre-layout information, ParaGraph (Ren et al. (2020)) builds a GNN model to predict layout-dependent parasitics and physical device parameters; GCN-RL circuit designer (Wang et al. (2020)) combines RL with GCNs for automatic transistor sizing. By using layout information, GNN surrogate models can predict the relative placement quality of different designs (Li et al. (2020c)), and other circuit properties, such as the electromagnetic properties of high-frequency circuits (Zhang et al. (2019a)).

B A BRIEF REVIEW OF MAGNETIC LAPLACIAN AND POSITIONAL ENCODINGS FOR DIRECTED GRAPHS

Positional encodings (PE) for graphs are vectorized representations that can effectively describe the global position of nodes (absolute PE) or relative position of node pairs (relative PE). They provide crucial positional information and thus benefits many backbone models that are position-agnostic. For instance, on undirected graphs, PE can provably alleviate the limited expressive power of Message Passing Neural Networks (Xu et al. (2019); Morris et al. (2019); Li et al. (2020b); Lim et al. (2022)); PE are also widely adopted in many graph transformers to incorporate positional information and break the identicalness of nodes in attention mechanism (Kreuzer et al. (2021); Ying et al. (2021); Rampásek et al. (2022); Chen et al. (2022)). As a result, the design and use of PE become one of the most important factors in building powerful graph encoders.

Likely, one can expect that direction-aware PE are also crucial when it comes to directed graph encoders. “Direction-aware” implies that PE should be able to capture the directedness of graphs. A notable example is Magnetic Laplacian PE (Geisler et al. (2023)), which adopts the eigenvectors of Magnetic Laplacian as PE. Note that Magnetic Laplacian can encode the directedness via the sign of phase of $\exp\{\pm i2\pi q\}$. Besides, when $q = 0$, Magnetic Laplacian reduces to normal symmetric Laplacian. Thus, Magnetic Laplacian PE for directed graphs can be seen as a generalization of Laplacian PE for undirected graphs, and the latter is known to enjoy many nice spectral properties (Chung (1997)) and be capable to capture many undirected graph distances (Kreuzer et al. (2021)). Therefore, Magnetic Laplacian appears to be a strong candidate for designing direction-aware PE. The definition is as follows:

Magnetic Laplacian (MagLap) matrix is a Hermitian complex matrix defined by $L_q = I - D^{-1/2} A_q D^{-1/2}$, where D is the diagonalized degree matrix counting both in-degree and out-degree, and A_q refers to the complex matrix as follows:

$$[A_q]_{u,v} = \begin{cases} \exp\{i2\pi q\}, & \text{if } (u, v) \in \mathcal{E}, \\ \exp\{-i2\pi q\}, & \text{if } (v, u) \in \mathcal{E}, \\ 1, & \text{if } (u, v), (v, u) \in \mathcal{E}, \end{cases} \quad (1)$$

with a parameter $q \in [0, 1)$ called potential. Hermitian refers to the property that complex conjugate L_q^\dagger equals to L_q . It is also worth noticing that when $q = 0$, MagLap $L_{q=0}$ degenerates to the standard symmetric Laplacian matrix $L = I - D^{-1/2}(A + A^\top)D^{-1/2}$ as a special case, where A is the Adjacency matrix. See Furutani et al. (2020) for a comprehensive introduction to Magnetic Laplacian.

Note that it is worth mentioning that there are also other PE for directed graphs, such as SVD of Adjacency matrix Hussain et al. (2022) and directed random walk Geisler et al. (2023).

C DATA SPLIT WHEN COMPARING WITH BASELINES IN THE ORIGINAL PAPERS

When comparing with the baselines from original papers, for training and testing the proposed new methods ‘BI-GINE+EPE’ and ‘BI-GPS+EPE’, we follow the dataset split of the original paper for fair comparison.

In the AMP dataset, we follow Dong et al. (2023) to merge the graphs with 2-stage and 3-stage Op-Amps together into one dataset, we take the last 1000 graphs for test and the rest for training and validation. The performance of baseline method cktGNN and the proposed new methods ‘BI-GINE+EPE’ and ‘BI-GPS+EPE’ are reported on such data split; for the HLS dataset, both the baseline method and the proposed new methods are trained and tested on control data flow graphs (CDFG) only, following the same data split ratio that randomly divide the data into training, validation and testing as described in the original paper Wu et al. (2022b); in the SR dataset, both the baseline and the new methods are trained with 24-bit netlists and tested on 48-bit netlists, note that both the training and testing data are obtained before technology mapping Wu et al. (2023); for the CG dataset both the baselines and the proposed methods are tested to predict the runtime of neural networks on the Cortex A76 CPU platform Zhang et al. (2021a); for the TIME dataset, we follow the dataset split in the original paper Guo et al. (2022) and compare the results of the baseline method and the new methods on the ID designs.

D DATASET SELECTION DETAILS

License for the datasets and codes.

	code implementation	dataset license
HLS Wu et al. (2022b)	MIT License	MIT License
AMP Dong et al. (2023)	MIT License	MIT License
SR Wu et al. (2023)	The MIT License	The MIT License
CG Zhang et al. (2021a)	MIT License	MIT License
our benchmark	CC BY-NC	- -

Table 7: License of the datasets and the toolbox implementation of this benchmark.

For detailed information of the license of each origin dataset, please refer to their original paper/documents, the final interpretation regarding the five dataset’s licensing information rests with the owner of the original paper. To the best of our knowledge, these hardware datasets contain no personally identifiable information or offensive content.

D.1 HIGH-LEVEL SYNTHESIS (HLS) DATASET

After HLS front-end compilation, six node features are extracted, as summarized in Table 8. Each edge has two features, the edge type represented in integers, and a binary value indicating whether this edge is a back edge. Each graph is labeled based on its post-implementation performance metrics, which are synthesized by Vitis HLS vit and implemented by Vivado viv. Three metrics are used for regression: DSP, LUT, and CP. The first two are integer numbers indicating the number of resources used in the final implementation; the last one is CP timing in fractional number, determining the maximum working frequency of FPGA. The DFG and CDFG datasets consists of 19,120 and 18,570 C programs, respectively. Figure 4 shows an example C program from the CDFG dataset, with the corresponding control dataflow graph shown in Figure 5. More information can be found in the original paper Wu et al. (2022b).

Feature	Description	Values
Node type	General node type	operation nodes, blocks, ports, misc
Bitwidth	Bitwidth of the node	0~256, misc
Opcode type	Opcode categories based on LLVM	binary_unary, bitwise, memory, etc.
Opcode	Opcode of the node	load, add, xor, icmp, etc.
Is start of path	Whether the node is the starting node of a path	0, 1, misc
Cluster group	Cluster number of the node	-1~256, misc

Table 8: Node features and their example values.

```

#include <stdio.h>
unsigned int fn(char p, float p_4, double p_6, unsigned int p_8)
{
    long v;
    unsigned int result;
    v = (long)p_6;
    if ((unsigned long)(-v) < 192523741UL)
        result = - ((unsigned int)((float)p - p_4) - 48507U);
    else {
        result = 4294963506U;
        result /= (unsigned int)(- p_6) * ! p_8 + 876U;
    }
    return result;
}

```

Figure 4: An example C program from the CDFG dataset.

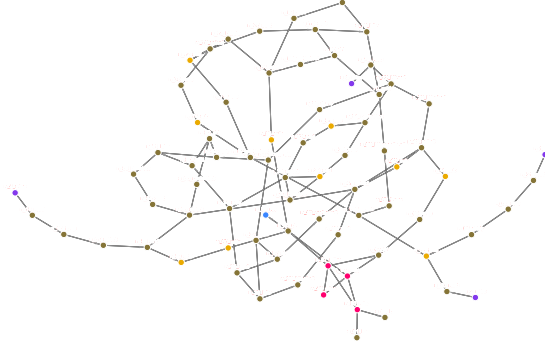


Figure 5: Control dataflow graph of the example program in Figure 4.

D.2 SYMBOLIC REASONING (SR) DATASET

In this dataset, all the circuit designs are represented as and-inverter graphs (AIGs), a concise and uniform representation of BNs consisting of inverters and two-input AND gates, which allows rewriting, simulation, technology mapping, placement, and verification to share the same data structure Mishchenko et al. (2006). In an AIG, each node has at most two incoming edges; a node without incoming edges is a primary input (PI); primary outputs (POs) are denoted by special output nodes; each internal node represents a two-input AND function. Based on De Morgan’s laws, any combinational BN can be converted into an AIG Brayton & Mishchenko (2010) in a fast and scalable manner.

For each node, there are three node features represented in binary values denoting node types and Boolean functionality. The first node feature indicates whether this node is a PI/PO or intermediate node (i.e., AND gate). The second and the third node features indicate whether each input edge is inverted or not, such that AIGs can be represented as homogeneous graphs without additional edge features.

This dataset aims to leverage graph learning based approaches to accelerate the adder tree extraction in (integer) multiplier verification, which involves two reasoning steps Li et al. (2013); Subramanyan et al. (2013): (1) detecting XOR/MAJ functions to construct adders, and then (2) identifying their boundaries. Thus, there are two sets of node labels, i.e., two node-level classification tasks. One task provides labels specifying whether a node (i.e., a gate) in the AIG belongs to MAJ, XOR, or is shared by both MAJ and XOR. The other task provides labels specifying whether a node is the root node of an adder. These AIGs and ground truth labels are generated by the logic synthesis tool ABC Brayton & Mishchenko (2010). Figure 6 shows the AIG of an 8-bit multiplier: the blue and red nodes are the root nodes of XOR functions, with the red nodes directly connecting to the POs; the green nodes are the root nodes of MAJ functions. By pairing one XOR function with one MAJ function sharing the same set of inputs, we can extract the adder tree, which is shown in Figure 7. More information can be found in the original paper Wu et al. (2023).

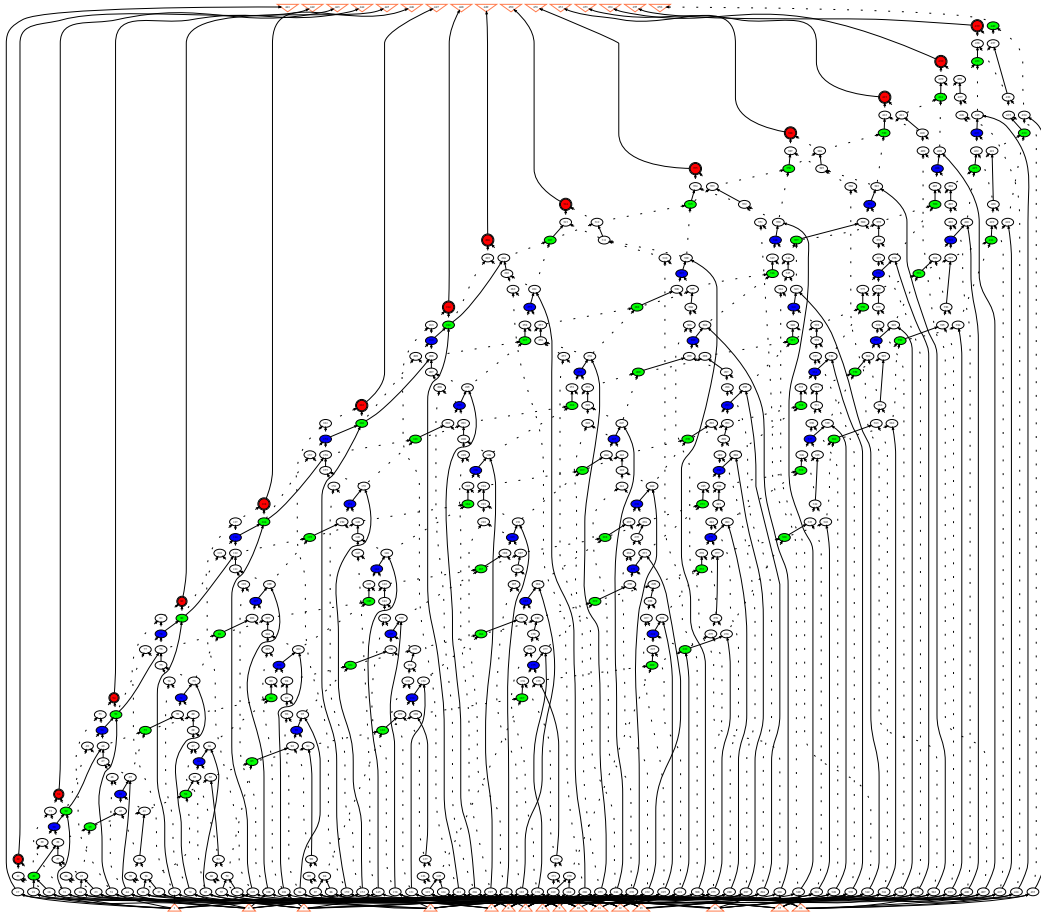


Figure 6: 8-bit multiplier in AIG.

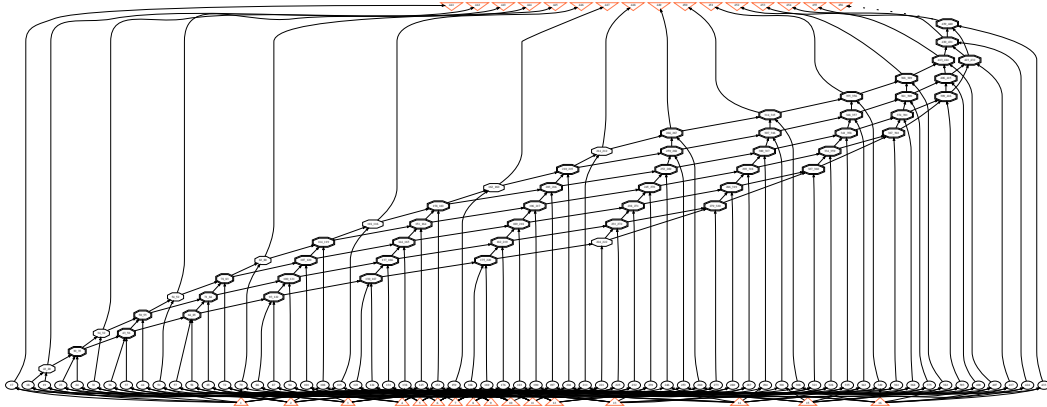


Figure 7: 8-bit multiplier with adders extracted.

D.3 PRE-ROUTING TIMING PREDICTION (TIME) DATASET

Similar to timing analysis tools, circuits in this dataset are represented as heterogeneous graphs consisting of two types of edges: net edges and cell edges, with edge features shown in Table 9a. The nodes in graphs denote pins in circuits, with features summarized in Table 9b. The TIME dataset collects 21 real-world benchmark circuits from OpenCores ope (a) with OpenROAD ope (b) on SkyWater 130nm technology sky (i.e. blabla, usb_cdc_core, BM64, salsa20, aes128, aes192,

Description	Size	Description	Size
(Net edge) Distances along x/y direction	2	Is primary I/O pin or not	1
(Cell edge) LUT is valid or no	8	Is fan-in or fan-out	1
(Cell) LUT indices	$8 \times (7 + 7)$	Distance to the 4 die area boundaries	4
(Cell) LUT value matrices	$8 \times (7 \times 7)$	Pin capacitance	4 (EL/RF)

(a) Edge features in the TIME dataset. For each cell edge, 8 LUTs are used to model cell delay and slew under four timing corner combinations (EL/RF).

(b) Pin (i.e., node) features in the TIME dataset. EL/RF stands for early/late and rise/fall, i.e., the four timing corner combinations in STA.

Table 9: Node and edge features for pre-routing timing prediction.

aes256, wqspiflash, cic_decimator, des, aes_cipher, picorv32a, zipdiv, genericfir, usb, jpeg_encoder, usbf_device, xtea, spm, y_huff, and synth_ram). More information can be found in the original paper Guo et al. (2022).

We select the slack prediction task in this dataset, including setup slack and hold slack. Slack values are used by STA tools to identify paths that violate timing constraints, enabling further optimization of placement and routing. Setup/hold slack is defined as the difference between the required arrival time (based on setup or hold time) and the actual arrival time of data/signals at timing endpoints, making it a node-level regression task.

Figure 8 shows the most common timing path, register-to-register path. (1) For setup slack, the signal should arrive *earlier* than the required arrival time (i.e., clock period - setup time). Setup time t_{setup} refers to the time before the clock edge that data must be stable. (2) For hold slack, the signal should arrive *later* than the required hold time to ensure no impact on signals for the current clock edge. Hold time t_{hold} refers to the time after the clock edge that data must be stable.

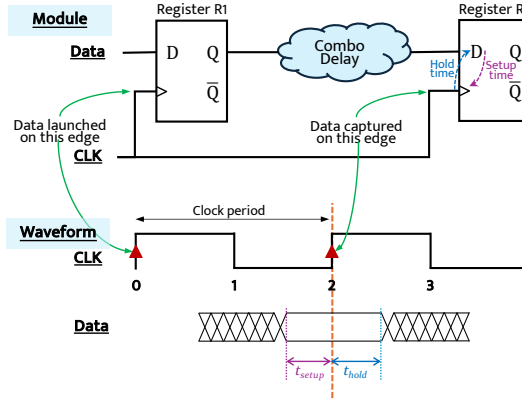


Figure 8: Register-to-register timing path.

D.3.1 TIME DATASET DISTRIBUTION SHIFT DEFINITION

For training and ID testing, we take the designs ‘blabla’, ‘usb_cdc_core’, ‘wbqspiflash’, ‘cic_decimator’, ‘picorv32a’, ‘zipdiv’, ‘usb’. For OOD testing, we use ‘xtea’, ‘spm’, ‘y_huff’, ‘synth_ram’.

D.4 COMPUTATIONAL GRAPH (CG) DATASET

This dataset includes (1) 12 state-of-the-art CNN models for the ImageNet2012 classification task (i.e., AlexNet, VGG, DenseNet, ResNet, SqueezeNet, GoogleNet, MobileNetv1, MobileNetv2, MobileNetv3, ShuffleNetv2, MnasNet, and ProxylessNas), each with 2,000 variants that differ in output channel number and kernel size per layer, and (2) 2,000 models from NASBench201 Dong & Yang (2019) with the highest test accuracy on CIFAR10, each featuring a unique set of edge connections. In total, this dataset contains 26,000 models with different operators and configurations. Figure 9 shows an example of the computational graph of a model in NASBench201.

Node features include input shape (5 dimensions), kernel/weight shape (padding to 4 dimensions), strides (2 dimensions), and output shape (5 dimensions). Each computational graph is labeled with the inference latency on three edge devices (i.e., Cortex A76 CPU, Adreno 630 GPU, Adreno 640 GPU). There is no edge feature in this dataset. More information can be found in the original paper Zhang et al. (2021a).

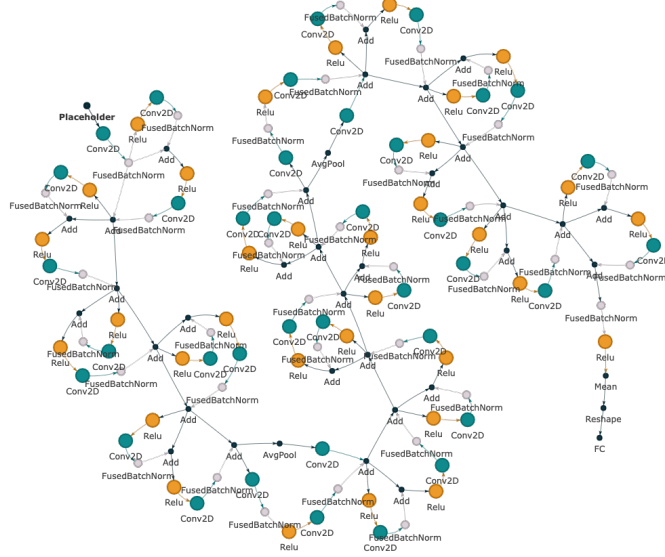


Figure 9: Computational graph of an example NN model from NASBench201 Dong & Yang (2019).

D.4.1 CG DATASET DISTRIBUTION SHIFT DEFINITION

For training and ID testing, we take ‘DenseNets’, ‘MnasNets’, ‘MobileNetv2s’, ‘MobileNetv3s’, ‘nasbench201s’. For OOD testing, we select ‘Proxylessnas’, ‘ResNets’, and ‘SqueezeNets’.

D.5 MULTI-STAGE AMPLIFIERS (AMP) DATASET

This dataset focuses on predicting circuit specifications (e.g., DC gain, bandwidth (BW), phase margin (PM)) of 2/3-stage operational amplifiers (Op-Amps), which are simulated by the circuit simulator Cadence Spectre spe. A 2/3-stage Op-Amp consists of (1) two/three single-stage Op-Amps on the main feedforward path and (2) several feedback paths, with one example shown in the right part of Figure 10. To make multi-stage Op-Amps more stable, feedforward and feedback paths are used to achieve different compensation schemes, each of which is implemented with a sub-circuit, e.g., single-stage Op-Amps, resistors, and capacitors. Due to the different topologies of single-stage Op-Amps and various compensation schemes, each sub-circuit is built as a subgraph. There are 24 potential sub-circuits in the considered 2/3-stage Op-Amps:

- Single R or C (① in Figure D.5, 2 types).
- R and C connected in parallel or serial (② in Figure D.5, 2 types).
- A single-stage Op-Amp (g_m) with different polarities (positive, $+g_m$, or negative, $-g_m$) and directions (feedforward or feedback) (③ in Figure D.5, 4 types).
- A single-stage Op-Amp (g_m) with R or C connected in parallel or serial (16 types). Note that we use the single-stage Op-Amp with feedforward direction and positive polarities as an example for ④ in Figure D.5.

Based on aforementioned formulation, node features include (1) subgraph type, (2) node type (e.g., R, C, $\pm g_m$ with feedforward/feedback, primary input/output), and (3) value of the component. There is no edge feature. More information can be found in the original paper Dong et al. (2023).

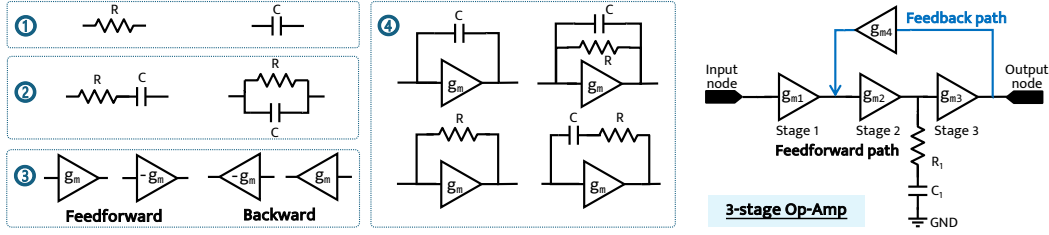


Figure 10: Subgraph basis for operational amplifiers and an example 3-stage Op-Amp.

E BENCHMARK DESIGN DETAILS

E.1 SELECTED BACKBONE FUNCTIONAL

Here we list the functions we implemented for the selected GNN backbone layers, note that here we show the forms of the backbone on undirected graphs, one may do slight modification by introducing $\omega(\cdot)$ on the neighbor message aggregation to consider message passing control for directed graphs.

$$\text{GIN} : \mathbf{x}_i^{(k)} = \text{MLP} \left(\mathbf{x}_i^{(k-1)} + \sum_{j \in \mathcal{N}(i)} \mathbf{x}_j^{(k-1)} \right) \quad (2)$$

is the for graphs without edge features,

$$\text{GINE} : \mathbf{x}_i^{(k)} = \text{MLP} \left(\mathbf{x}_i^{(k-1)} + \sum_{j \in \mathcal{N}(i)} \text{ReLU}(\mathbf{x}_j^{(k-1)} + \mathbf{e}_{j,i}^{(k-1)}) \right) \quad (3)$$

is used for graphs with edge features.

$$\text{GCN} : \mathbf{x}_i^{(k)} = \theta^\top \sum_{j \in \mathcal{N}(i) \cup \{i\}} \frac{\mathbf{e}_{j,i}^{(k-1)}}{\sqrt{\hat{d}_j \hat{d}_i}} \mathbf{x}_j^{(k-1)}, \quad (4)$$

where θ is the parameter to learn, for graphs with edge features $\mathbf{e}_{j,i}$ is the processed edge weight, for graphs without edge features $\mathbf{e}_{j,i}$ is set as 1.

$$\text{GAT} : \mathbf{x}_i^{(k)} = \alpha_{i,i}^{(k-1)} \theta_s \mathbf{x}_i^{(k-1)} + \sum_{j \in \mathcal{N}(i)} \alpha_{i,j}^{(k-1)} \theta_t \mathbf{x}_j^{(k-1)}, \quad (5)$$

where θ_s, θ_t are parameters to learn, for graphs without edge features,

$$\alpha_{i,j}^{(k-1)} = \frac{\exp \left(\text{LeakyReLU} \left(\mathbf{a}_s^\top \theta_s \mathbf{x}_i^{(k-1)} + \mathbf{a}_t^\top \theta_t \mathbf{x}_j^{(k-1)} \right) \right)}{\sum_{m \in \mathcal{N}(i) \cup \{i\}} \exp \left(\text{LeakyReLU} \left(\mathbf{a}_s^\top \theta_s \mathbf{x}_i^{(k-1)} + \mathbf{a}_t^\top \theta_t \mathbf{x}_m^{(k-1)} \right) \right)}, \quad (6)$$

and for graphs with edge features,

$$\alpha_{i,j}^{(k-1)} = \frac{\exp \left(\text{LeakyReLU} \left(\mathbf{a}_s^\top \theta_s \mathbf{x}_i^{(k-1)} + \mathbf{a}_t^\top \theta_t \mathbf{x}_j^{(k-1)} + \mathbf{a}_e^\top \theta_e \mathbf{e}_{i,j}^{(k-1)} \right) \right)}{\sum_{m \in \mathcal{N}(i) \cup \{i\}} \exp \left(\text{LeakyReLU} \left(\mathbf{a}_s^\top \theta_s \mathbf{x}_i^{(k-1)} + \mathbf{a}_t^\top \theta_t \mathbf{x}_m^{(k-1)} + \mathbf{a}_e^\top \theta_e \mathbf{e}_{i,m}^{(k-1)} \right) \right)}, \quad (7)$$

where $\mathbf{a}_s, \mathbf{a}_t$ are learnable parameterized attention parameters.

Each GPS backbone layer is implemented as follows:

$$\begin{aligned} \text{GPS} : \mathbf{X}_M^{(k)} &= \text{MPNN}^{(k-1)}(\mathbf{X}^{(k-1)}, \mathbf{E}^{(k-1)}) \\ \mathbf{X}_T^{(k)} &= \text{GlobalATTn}^{(k-1)}(\mathbf{X}^{(k-1)}) \\ \mathbf{X}^{(k)} &= \text{MLP}(\mathbf{X}_M^{(k-1)} + \mathbf{X}_T^{(k-1)}), \end{aligned} \quad (8)$$

where \mathbf{X}, \mathbf{E} denote node/edge features, we use GIN or GINE as the MPNN layer, and we use the transformer as the global attention reasoning layer.

For DGCN Tong et al. (2020b) and DiGCN Tong et al. (2020a), we follow the implementation in PyGSD He et al. (2024), please refer to <https://pytorch-geometric-signed-directed.readthedocs.io/en/latest/index.html> for backbone implementation details.

$$\text{MSGNN: } \mathbf{x}_i^{(k)} = \sigma \left(\sum_{j=1}^{F^{k-1}} \mathbf{Y}_{ij} \mathbf{x}_j^{(k-1)} + \mathbf{b}_j^{(k-1)} \right), \quad (9)$$

where σ is a complex version of Rectified Linear Unit defined by:

$$\sigma(z) = \begin{cases} z & -\pi/2 \leq \arg(z) < \pi/2 \\ 0 & \text{otherwise,} \end{cases}$$

where $\arg(\cdot)$ is the complex argument of $z \in \mathbb{C}$, $F^{(k)}$ denotes the number of channels in the k -th layer, \mathbf{b} is a bias vector with equal real and imaginary parts, \mathbf{Y} denotes the convolution matrix defined in Equation.(4) and (5) in He et al. (2022).

E.2 HYPER-PARAMETER SPACE

	batch size	learning rate	dropout rate	hidden dimension*	# of GNN layers	# of MLP layers
DGCN	{64, 128, 256, 512, 1024}	[5e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 336]	[3,8]	[2,5]
DiGCN	{64, 128, 256, 512, 1024}	[5e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 336]	[3,8]	[2,5]
MagNet	{64, 128, 256, 512, 1024}	[5e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 336]	[3,8]	[2,5]
GCN	{64, 128, 256, 512, 1024}	[1e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 336]	[3,8]	[2,5]
GIN	{64, 128, 256, 512, 1024}	[1e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 336]	[3,8]	[2,5]
GAT	{64, 128, 256, 512, 1024}	[1e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 336]	[3,8]	[2,5]
GPS-T	{64, 128, 256}	[1e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 288]	[3,6]	[2,5]
GPS-P	{32, 64, 128, 256, 512}	[1e-4, 1e-2]	{0, 0.1, 0.2, 0.3}	[96, 288]	[3,6]	[2,5]

Table 10: Hyper-parameter space for each backbone. *:hidden dimension slightly vary in each task.

F HARDWARE AND PLATFORM

All the experiments run on a server with an AMP EPYC 7763 64-Core Processor and 8 Nvidia RTX6000 GPU cards. The codes run on frameworks based on PyTorch Paszke et al. (2019), PyTorch Geometric Fey & Lenssen (2019), PyTorch Geometric Signed and Directed He et al. (2024), RAY Liaw et al. (2018).

G IMPLEMENTATION DETAILS OF EXPERIMENTS

G.1 RANKING CALCULATION

In Table. 4 and Table. 3, we report the average ranking of different combination of methods w.r.t. per evaluation metrics for each task from each dataset. The calculation of the ranking can be expressed as:

$$\text{rank}_k^{t,D} = \frac{1}{M_D} \sum_{m=1}^{M_D} R_{t,m}^k, \quad (10)$$

where $R_{t,m}^k$ denotes the ranking of the DGRL method k on task t w.r.t. the m -th evaluation metric. M_D denotes the number of tasks and metrics on dataset D .

For evaluation metric the larger the better, we adopt the ranking function from pandas pandas development team (2020) with parameter *ascending* = *False* and *method* = '*max*'.

For evaluation metrics the smaller the better, we use *ascending* = *True* and *method* = '*min*'.

H DETAILED EXPERIMENT RESULTS

H.1 MAIN RESULTS: IN-DISTRIBUTION AND OUT-OF-DISTRIBUTION PERFORMANCE

Method	shared				root			
	accuracy	precision	recall	f1	accuracy	precision	recall	f1
GCN	0.879±0.013	0.669±0.141	0.653±0.125	0.620±0.119	0.882±0.005	0.860±0.045	0.811±0.131	0.773±0.091
DI-GCN	0.633±0.000	0.376±0.000	0.377±0.000	0.337±0.000	0.751±0.000	0.250±0.000	0.333±0.000	0.285±0.000
BI-GCN	0.992±0.005	0.816±0.123	0.820±0.122	0.818±0.123	0.999±0.001	0.999±0.000	0.998±0.003	0.999±0.001
GIN	0.882±0.046	0.787±0.132	0.704±0.191	0.683±0.179	0.909±0.005	0.900±0.055	0.877±0.101	0.850±0.050
DI-GIN	0.999±0.000	0.749±0.000	0.749±0.000	0.749±0.000	0.999±0.000	0.999±0.000	0.999±0.000	0.999±0.000
BI-GIN	0.999±0.000	0.937±0.088	0.974±0.079	0.949±0.080	0.999±0.000	0.999±0.000	0.999±0.000	0.999±0.000
GAT	0.881±0.003	0.626±0.074	0.571±0.083	0.539±0.073	0.877±0.007	0.821±0.074	0.825±0.126	0.786±0.090
DI-GAT	0.885±0.060	0.679±0.033	0.682±0.034	0.674±0.036	0.981±0.005	0.985±0.009	0.956±0.012	0.970±0.008
BI-GAT	0.984±0.034	0.941±0.108	0.939±0.108	0.940±0.108	0.998±0.002	0.996±0.006	0.998±0.003	0.997±0.004
GPS-P	0.895±0.002	0.899±0.031	0.845±0.066	0.829±0.051	0.893±0.002	0.888±0.047	0.837±0.121	0.806±0.071
DI-GPS-P	0.999±0.000	0.749±0.000	0.749±0.000	0.749±0.000	0.999±0.000	0.999±0.000	0.999±0.000	0.999±0.000
BI-GPS-P	0.997±0.002	0.747±0.003	0.748±0.001	0.748±0.002	0.994±0.003	0.997±0.001	0.986±0.008	0.991±0.005
DGCN	0.975±0.000	0.734±0.000	0.730±0.000	0.732±0.000	0.991±0.000	0.989±0.003	0.984±0.003	0.987±0.000
DiGCN	0.995±0.000	0.747±0.000	0.747±0.000	0.747±0.000	0.994±0.001	0.990±0.007	0.991±0.004	0.991±0.004
MagNet	0.999±0.000	1.000±0.000	1.000±0.000	1.000±0.000	0.999±0.000	1.000±0.000	1.000±0.000	1.000±0.000

Table 11: ID performance on the SR dataset.

Method	gain		PM		BW	
	mse	rmse	mse	rmse	mse	rmse
GCN	1.262±1.682	0.993±0.554	13.598±30.906	2.618±2.736	35.230±0.657	5.935±0.055
DI-GCN	0.337±0.002	0.580±0.002	1.243±0.014	1.115±0.006	36.302±0.245	6.025±0.020
BI-GCN	0.148±0.004	0.385±0.005	63.874±194.025	3.862±7.375	22.947±1.022	4.789±0.105
GIN	0.166±0.029	0.406±0.034	1.266±0.034	1.125±0.015	28.259±10.648	5.244±0.894
DI-GIN	0.200±0.136	0.433±0.117	1.300±0.024	1.140±0.010	24.091±1.270	4.906±0.130
BI-GIN	0.137±0.012	0.370±0.016	1.251±0.035	1.118±0.016	19.724±1.489	4.438±0.170
GAT	0.158±0.008	0.397±0.010	865.339±2684.901	11.663±28.466	22.770±1.045	4.770±0.111
DI-GAT	0.205±0.006	0.453±0.007	1.562±0.840	1.223±0.268	26.855±2.928	5.175±0.284
BI-GAT	0.138±0.007	0.372±0.010	1.213±0.055	1.101±0.024	30.333±13.386	5.409±1.088
GPS-T	0.405±0.022	0.636±0.017	1.277±0.072	1.129±0.031	16.758±0.754	4.092±0.093
DI-GPS-T	0.122±0.009	0.349±0.013	1.259±0.044	1.121±0.019	16.600±0.877	4.073±0.107
BI-GPS-T	0.122±0.007	0.349±0.010	1.212±0.058	1.100±0.026	20.475±8.853	4.456±0.825
DGCN	0.567±0.004	0.753±0.003	1.292±0.000	1.136±0.000	54.256±0.257	7.365±0.017
DiGCN	0.367±0.009	0.606±0.007	1.294±0.011	1.137±0.005	52.375±0.276	7.237±0.019
MagNet	0.185±0.008	0.431±0.009	1.315±0.082	1.146±0.035	24.800±2.834	4.972±0.283

Table 12: ID performance on the AMP dataset.

Method	DSP		LUT		CP	
	mse	R2	mse	R2	mse	R2
GCN	12.700±0.324	0.877±0.004	4.909±0.123	0.647±0.021	0.713±0.037	0.829±0.012
DI-GCN	12.591±0.312	0.877±0.003	4.998±0.114	0.643±0.013	0.692±0.013	0.837±0.004
BI-GCN	10.285±0.336	0.902±0.004	4.311±0.149	0.732±0.010	0.665±0.025	0.847±0.007
GINE	2.707±0.133	0.975±0.001	2.172±0.108	0.861±0.008	0.653±0.014	0.849±0.003
DI-GINE	2.312±0.172	0.979±0.001	2.145±0.158	0.863±0.011	0.645±0.022	0.851±0.007
BI-GINE	2.137±0.076	0.981±0.000	1.759±0.087	0.892±0.005	0.629±0.020	0.855±0.005
GAT	4.680±0.264	0.957±0.002	3.267±0.142	0.778±0.011	0.643±0.012	0.850±0.004
DI-GAT	7.697±0.238	0.926±0.002	4.188±0.226	0.685±0.031	0.677±0.051	0.840±0.014
BI-GAT	4.718±0.532	0.957±0.004	3.028±0.143	0.801±0.016	0.590±0.011	0.863±0.006
GPS	2.444±0.207	0.978±0.002	2.114±0.153	0.872±0.011	0.621±0.028	0.858±0.010
DI-GPS	2.517±0.180	0.977±0.001	2.306±0.224	0.862±0.015	0.625±0.028	0.856±0.007
BI-GPS	2.442±0.303	0.979±0.002	2.112±0.216	0.873±0.014	0.621±0.018	0.859±0.009
DGCN	19.614±1.151	0.816±0.010	7.988±2.512	0.333±0.256	1.127±0.049	0.706±0.014
DiGCN	12.125±0.204	0.885±0.003	5.683±0.638	0.527±0.092	0.704±0.019	0.836±0.004
MagNet	4.375±0.452	0.961±0.003	2.381±0.175	0.848±0.015	0.684±0.045	0.843±0.014

Table 13: ID performance on the HLS dataset.

Method	shared				root			
	accuracy	precision	recall	f1	accuracy	precision	recall	f1
GCN	0.510±0.021	0.283±0.014	0.328±0.018	0.292±0.016	0.569±0.056	0.364±0.069	0.317±0.038	0.321±0.038
DI-GCN	0.553±0.000	0.318±0.000	0.374±0.000	0.301±0.000	0.741±0.000	0.247±0.000	0.333±0.000	0.283±0.000
BI-GCN	0.671±0.045	0.489±0.035	0.563±0.045	0.513±0.037	0.651±0.054	0.512±0.057	0.514±0.064	0.505±0.062
GIN	0.677±0.039	0.414±0.034	0.395±0.064	0.371±0.067	0.743±0.008	0.646±0.084	0.378±0.027	0.367±0.045
DI-GIN	0.621±0.027	0.449±0.047	0.462±0.024	0.441±0.026	0.729±0.010	0.475±0.047	0.390±0.079	0.371±0.082
BI-GIN	0.712±0.024	0.514±0.040	0.561±0.071	0.500±0.049	0.773±0.018	0.592±0.070	0.502±0.051	0.515±0.054
GAT	0.583±0.118	0.341±0.062	0.383±0.071	0.343±0.079	0.633±0.088	0.456±0.065	0.435±0.043	0.408±0.055
DI-GAT	0.547±0.061	0.384±0.032	0.453±0.072	0.394±0.038	0.642±0.041	0.431±0.062	0.474±0.061	0.437±0.058
BI-GAT	0.554±0.078	0.416±0.069	0.450±0.080	0.397±0.072	0.632±0.046	0.483±0.066	0.477±0.065	0.461±0.061
GPS-P	0.670±0.059	0.407±0.055	0.454±0.056	0.404±0.047	0.659±0.040	0.395±0.056	0.410±0.045	0.385±0.037
DI-GPS-P	0.651±0.059	0.421±0.053	0.499±0.056	0.441±0.050	0.665±0.077	0.441±0.059	0.509±0.088	0.450±0.065
BI-GPS-P	0.651±0.057	0.417±0.040	0.482±0.040	0.435±0.045	0.671±0.023	0.491±0.020	0.578±0.049	0.507±0.029
DGCN	0.628±0.009	0.497±0.028	0.391±0.043	0.400±0.045	0.709±0.020	0.511±0.035	0.495±0.024	0.498±0.028
DiGCN	0.470±0.094	0.432±0.031	0.493±0.040	0.396±0.056	0.726±0.016	0.505±0.023	0.501±0.013	0.497±0.017
MagNet	0.703±0.040	0.445±0.047	0.499±0.052	0.463±0.046	0.683±0.032	0.457±0.057	0.413±0.045	0.413±0.043

Table 14: OOD performance on the SR dataset.

Method	gain		pm		bw	
	mse	rmse	mse	rmse	mse	rmse
GCN	0.877±1.063	0.856±0.399	101.444±308.123	4.823±9.320	42.921±0.993	6.551±0.075
DI-GCN	0.451±0.015	0.671±0.011	1.412±0.012	1.188±0.005	46.374±0.590	6.809±0.043
BI-GCN	0.270±0.036	0.519±0.033	21.490±58.748	2.861±3.844	30.004±2.192	5.474±0.201
GIN	0.337±0.041	0.580±0.034	1.436±0.053	1.198±0.022	34.398±11.114	5.806±0.852
DI-GIN	0.356±0.071	0.594±0.055	1.379±0.015	1.174±0.006	44.154±12.707	6.584±0.941
BI-GIN	0.293±0.026	0.541±0.024	1.419±0.046	1.191±0.019	25.822±1.977	5.078±0.190
GAT	0.330±0.032	0.574±0.027	567.911±1750.531	9.859±22.869	30.155±1.879	5.489±0.169
DI-GAT	0.412±0.035	0.641±0.027	1.406±0.078	1.185±0.032	41.750±10.476	6.421±0.753
BI-GAT	0.198±0.012	0.445±0.014	1.348±0.052	1.160±0.022	41.008±13.522	6.336±0.976
GPS-T	0.508±0.059	0.712±0.041	1.415±0.061	1.189±0.025	21.815±1.973	4.666±0.206
DI-GPS-T	0.301±0.012	0.549±0.011	1.447±0.037	1.202±0.015	22.161±1.355	4.705±0.144
BI-GPS-T	0.314±0.030	0.560±0.027	1.315±0.050	1.146±0.021	26.607±10.277	5.087±0.897
DGCN	0.772±0.046	0.878±0.025	1.364±0.000	1.168±0.000	69.019±1.345	8.307±0.081
DiGCN	0.345±0.014	0.587±0.012	1.377±0.021	1.173±0.009	59.337±0.659	7.703±0.042
MagNet	0.285±0.065	0.531±0.059	1.608±0.127	1.267±0.051	36.505±2.749	6.038±0.227

Table 15: OOD performance on the AMP dataset.

Method	DSP		LUT		CP	
	mse	R2	mse	R2	mse	R2
GCN	10.817±0.284	0.878±0.006	0.440±0.084	0.879±0.022	0.559±0.033	0.784±0.014
DI-GCN	11.101±0.468	0.873±0.006	0.454±0.128	0.863±0.053	0.593±0.009	0.774±0.006
BI-GCN	9.996±0.319	0.884±0.007	0.627±0.158	0.857±0.026	0.514±0.019	0.803±0.013
GINE	3.720±0.154	0.961±0.001	0.129±0.042	0.966±0.009	0.491±0.017	0.809±0.008
DI-GINE	3.194±0.122	0.967±0.001	0.118±0.022	0.968±0.005	0.513±0.025	0.804±0.015
BI-GINE	3.244±0.102	0.966±0.001	0.110±0.029	0.971±0.007	0.476±0.027	0.815±0.011
GAT	5.440±0.271	0.941±0.003	0.368±0.054	0.900±0.015	0.496±0.019	0.809±0.007
DI-GAT	8.927±0.355	0.895±0.005	0.456±0.135	0.856±0.040	0.551±0.034	0.784±0.015
BI-GAT	5.418±0.305	0.942±0.003	0.218±0.054	0.938±0.023	0.466±0.026	0.821±0.013
GPS	3.343±0.147	0.966±0.001	0.145±0.026	0.962±0.007	0.543±0.124	0.793±0.024
DI-GPS	3.210±0.146	0.967±0.001	0.139±0.032	0.964±0.008	0.461±0.016	0.820±0.014
BI-GPS	3.209±0.263	0.967±0.001	0.133±0.027	0.968±0.006	0.496±0.017	0.812±0.016
DGCN	20.220±1.474	0.756±0.024	0.647±0.228	0.797±0.095	1.159±0.093	0.519±0.028
DiGCN	10.922±0.353	0.880±0.004	0.665±0.257	0.758±0.098	0.613±0.022	0.770±0.011
MagNet	5.048±0.499	0.947±0.004	0.168±0.049	0.955±0.012	0.557±0.053	0.793±0.024

Table 16: OOD performance on the HLS dataset.

Method	blabla	usb_cdc_core	wbqspiflash	cic_decimator	picorv32a	zipdiv	usb	average
GCN	9.263±1.994	2.888±0.576	0.382±0.266	0.684±0.151	8.796±1.773	8.796±1.773	0.501±0.076	3.278±0.318
DI-GCN	13.008±5.156	2.764±0.347	0.504±0.245	0.594±0.293	10.166±2.557	10.166±2.557	0.622±0.087	4.058±0.892
BI-GCN	0.731±0.143	1.308±0.559	0.091±0.044	0.069±0.027	1.447±0.198	1.447±0.198	0.093±0.058	0.575±0.108
GINE	0.183±0.023	0.073±0.014	0.027±0.005	0.009±0.003	0.549±0.033	0.549±0.033	0.024±0.005	0.125±0.008
DI-GINE	1.133±0.156	0.166±0.041	0.147±0.041	0.048±0.024	1.361±0.398	1.361±0.398	0.123±0.051	0.439±0.048
BI-GINE	0.142±0.014	0.111±0.083	0.023±0.006	0.010±0.005	0.574±0.041	0.574±0.041	0.032±0.013	0.132±0.012
GAT	17.032±16.149	3.128±0.521	0.477±0.603	0.393±0.219	6.910±3.546	6.910±3.546	0.448±0.296	4.204±3.054
DI-GAT	61.647±17.523	3.359±0.563	1.728±0.436	0.756±0.270	14.218±3.930	14.218±3.930	0.746±0.155	12.295±3.179
BI-GAT	1.311±0.435	1.291±0.466	0.213±0.104	0.221±0.059	2.065±0.507	2.065±0.507	0.258±0.078	0.787±0.112
GPS-P	0.415±0.091	1.846±0.170	0.204±0.055	0.140±0.064	2.308±0.084	2.308±0.084	0.078±0.017	0.772±0.036
DI-GPS-P	0.334±0.091	0.283±0.110	0.160±0.049	0.105±0.029	1.973±0.093	1.973±0.093	0.051±0.011	0.440±0.028
BI-GPS-P	3.469±0.531	1.786±0.606	0.389±0.251	0.283±0.412	3.908±0.344	3.908±0.344	0.172±0.169	1.544±0.294
DGCN	104.383±0.123	4.278±0.152	2.314±0.032	1.262±0.045	19.884±0.203	19.884±0.203	1.586±0.073	19.933±0.049
DiGCN	47.858±14.097	4.134±0.429	1.725±0.426	1.011±0.324	13.460±1.900	13.460±1.900	1.086±0.306	10.547±2.441
MagNet	12.326±5.494	3.738±0.707	0.576±0.159	0.569±0.302	5.715±1.130	5.715±1.130	0.539±0.239	3.459±0.782

Table 17: ID performance with ‘mse’ metric on the Time dataset to predict hold slack.

Method	blabla	usb_cdc_core	wbqspiflash	cic_decimator	picorv32a	zipdiv	usb	average
GCN	0.910±0.019	-0.312±0.262	0.826±0.120	0.358±0.142	0.460±0.108	0.905±0.029	0.539±0.070	0.526±0.045
DI-GCN	0.873±0.050	-0.255±0.157	0.771±0.110	0.442±0.275	0.376±0.156	0.835±0.070	0.428±0.079	0.496±0.056
BI-GCN	0.992±0.001	0.405±0.254	0.958±0.020	0.935±0.025	0.911±0.012	0.937±0.011	0.914±0.053	0.865±0.047
GINE	0.998±0.000	0.966±0.006	0.987±0.002	0.991±0.003	0.966±0.002	0.997±0.001	0.977±0.004	0.983±0.001
DI-GINE	0.988±0.001	0.924±0.018	0.933±0.018	0.954±0.022	0.916±0.024	0.978±0.002	0.886±0.047	0.940±0.007
BI-GINE	0.998±0.000	0.949±0.037	0.989±0.002	0.990±0.005	0.964±0.002	0.993±0.005	0.970±0.012	0.979±0.006
GAT	0.834±0.156	-0.421±0.236	0.784±0.272	0.630±0.205	0.575±0.217	0.772±0.230	0.588±0.271	0.537±0.168
DI-GAT	0.401±0.170	-0.526±0.255	0.218±0.197	0.290±0.253	0.127±0.241	0.209±0.165	0.314±0.142	0.147±0.143
BI-GAT	0.987±0.004	0.413±0.212	0.903±0.047	0.792±0.055	0.873±0.031	0.966±0.017	0.762±0.072	0.814±0.033
GPS-P	0.996±0.000	0.020±0.090	0.881±0.032	0.907±0.042	0.839±0.005	0.903±0.024	0.925±0.016	0.782±0.014
DI-GPS-P	0.996±0.000	0.856±0.055	0.941±0.018	0.881±0.033	0.857±0.006	0.951±0.028	0.927±0.016	0.916±0.017
BI-GPS-P	0.968±0.004	0.052±0.321	0.773±0.146	0.814±0.270	0.727±0.023	0.812±0.178	0.837±0.159	0.712±0.136
DGCN	-0.013±0.001	-0.943±0.069	-0.046±0.014	-0.183±0.042	-0.220±0.012	-0.276±0.026	-0.455±0.067	-0.305±0.029
DiGCN	0.535±0.136	-0.877±0.195	0.219±0.192	0.050±0.304	0.173±0.116	0.002±0.239	0.003±0.280	0.015±0.169
MagNet	0.880±0.053	-0.698±0.321	0.739±0.071	0.465±0.283	0.649±0.069	0.836±0.080	0.505±0.220	0.482±0.055
Timer-inspired GNN	0.9616	0.9751	0.9721	0.9840	0.9688	0.9753	0.9784	0.9736

Table 18: ID performance with ‘R2’ metric on the Time dataset to predict hold slack.

Method	blabla	usb_cdc_core	wbqspiflash	cic_decimator	picorv32a	zipdiv	usb	average
GCN	127.555±9.301	17.551±1.646	34.125±1.436	1.399±0.128	126.288±10.077	28.960±1.970	17.849±1.509	50.532±1.053
DI-GCN	99.699±13.849	18.302±5.510	30.164±2.874	2.984±4.527	135.526±16.281	26.859±5.355	15.223±4.432	46.965±2.204
BI-GCN	104.062±11.187	12.867±1.746	27.941±1.197	4.693±0.572	102.680±9.184	20.688±1.020	6.033±2.329	39.852±2.405
GINE	24.911±9.848	2.819±0.801	8.012±3.029	1.233±0.360	31.441±2.463	3.379±1.141	2.211±0.517	10.572±0.027
DI-GINE	25.642±6.938	2.207±0.586	7.105±2.635	1.823±0.632	21.690±1.080	4.088±1.363	1.785±0.315	9.191±1.564
BI-GINE	21.108±6.326	1.690±0.510	4.484±1.648	1.079±0.778	23.207±5.134	3.160±2.036	2.695±2.925	8.203±1.720
GAT	105.449±39.675	13.554±3.935	32.138±2.692	3.416±1.475	116.730±16.637	25.274±2.653	7.188±2.344	43.393±3.497
DI-GAT	94.262±14.843	14.390±2.879	44.365±4.951	2.265±1.418	94.712±6.261	25.569±3.563	7.875±3.932	40.491±1.637
BI-GAT	68.198±12.533	14.929±2.209	21.334±2.564	3.263±0.779	76.571±9.852	19.570±1.516	4.016±1.470	29.697±2.690
GPS-P	71.180±7.296	6.017±0.951	19.114±3.978	2.786±0.931	40.219±2.599	21.280±5.284	1.974±0.394	23.224±2.482
DI-GPS-P	76.600±6.188	6.559±2.542	22.725±1.503	15.529±9.577	39.556±2.732	23.995±3.420	4.789±1.457	27.107±0.881
BI-GPS-P	79.395±9.864	6.205±1.437	21.067±5.043	4.882±1.370	39.426±3.651	26.285±4.810	3.748±0.912	25.858±2.168
DGCN	84.413±11.949	5.364±1.023	21.575±3.172	4.393±2.014	40.810±3.904	27.617±4.680	3.125±1.675	26.757±1.564
DiGCN	1790.553±159.661	68.846±51.069	86.761±47.738	33.962±17.288	546.052±1206.931	73.563±40.920	52.554±32.869	378.899±320.555
MagNet	106.479±18.775	7.917±0.623	25.831±1.098	11.474±0.993	131.028±12.043	15.074±0.966	4.877±0.662	43.240±2.216

Table 19: ID performance with ‘R2’ metric on the Time dataset to predict setup slack.

Method	blabla	usb_cdc_core	wbqspiflash	cic_decimator	picorv32a	zipdiv	usb	average
GCN	-1.030±0.148	-4.397±0.506	-0.219±0.051	0.180±0.075	-2.489±0.278	-0.971±0.134	-4.437±0.459	-1.909±0.150
DI-GCN	-0.586±0.220	-4.628±1.694	-0.077±0.102	-0.747±2.650	-2.744±0.449	-0.828±0.364	-3.637±1.350	-1.892±0.254
BI-GCN	-0.656±0.178	-2.956±0.537	0.001±0.042	-1.747±0.335	-1.837±0.253	-0.408±0.069	-0.837±0.709	-1.206±0.144
GINE	0.603±0.156	0.132±0.246	0.713±0.108	0.278±0.211	0.131±0.068	0.769±0.077	0.326±0.157	0.422±0.078
DI-GINE	0.591±0.110	0.321±0.180	0.746±0.101	-0.067±0.370	0.400±0.029	0.721±0.092	0.456±0.096	0.452±0.055
BI-GINE	0.664±0.100	0.480±0.157	0.839±0.058	0.367±0.455	0.358±0.141	0.784±0.138	0.178±0.891	0.524±0.183
GAT	-0.678±0.631	-3.168±1.210	-0.148±0.096	-1.000±0.863	-2.225±0.459	-0.720±0.180	-1.189±0.714	-1.304±0.175
DI-GAT	-0.500±0.236	-3.425±0.885	-0.585±0.176	-0.326±0.830	-1.617±0.173	-0.740±0.242	-1.399±1.197	-1.227±0.120
BI-GAT	-0.085±0.199	-3.591±0.679	0.237±0.091	-0.910±0.456	-1.115±0.272	-0.332±0.103	-0.223±0.447	-0.860±0.174
GPS-P	-0.091±0.111	-0.121±0.177	0.010±0.205	-0.313±0.439	0.034±0.062	-0.056±0.262	0.207±0.158	-0.047±0.151
DI-GPS-P	-0.071±0.086	-0.339±0.519	-0.076±0.071	-6.422±4.577	-0.052±0.072	-0.208±0.172	-0.591±0.484	-1.108±0.654
BI-GPS-P	-0.217±0.151	-0.156±0.267	-0.090±0.261	-1.302±0.645	0.053±0.087	-0.304±0.238	-0.504±0.366	-0.360±0.168
DGCN	-0.294±0.183	0.000±0.190	-0.116±0.164	-1.071±0.949	0.020±0.093	-0.370±0.232	-0.254±0.672	-0.298±0.243
DiGCN	-27.500±18.458	-20.171±15.704	-2.100±1.705	-18.882±10.121	-14.088±33.349	-4.007±2.785	-15.008±10.012	-14.537±8.681
MagNet	-0.694±0.298	-1.434±0.191	0.076±0.309	-5.717±0.581	-2.620±0.332	-0.026±0.065	-0.485±0.201	-1.557±0.090

Table 20: ID performance with ‘R2’ metric on the Time dataset to predict setup slack.

Method	hold				setup			
	xtea		synth_ram		xtea		synth_ram	
	mse	r2	mse	r2	mse	r2	mse	r2
GCN	6.745±0.853	-0.062±0.134	7.511±1.387	-1.030±0.375	117.599±4.681	-2.963±0.157	509.769±16.052	-984.202±31.023
DI-GCN	7.010±0.592	-0.104±0.093	9.764±2.355	-1.640±0.636	116.332±16.048	-2.920±0.540	418.819±24.262	-808.427±46.890
BI-GCN	5.675±0.784	0.105±0.123	2.446±0.255	0.338±0.069	100.915±4.158	-2.401±0.140	371.644±10.433	-717.255±20.164
GINE	4.446±1.623	0.299±0.255	2.482±1.650	0.328±0.446	62.927±28.904	-1.120±0.974	1341.500±430.261	-2591.639±831.541
DI-GINE	3.075±0.887	0.515±0.139	9.545±4.222	-1.581±1.141	61.694±6.981	-1.079±0.235	612.807±101.175	-1183.337±195.535
BI-GINE	2.116±0.486	0.666±0.076	1.314±1.197	0.644±0.323	83.775±17.953	-1.823±0.605	498.357±239.343	-962.146±462.565
GAT	7.446±1.012	-0.173±0.159	7.741±1.932	-1.093±0.522	96.486±7.970	-2.251±0.268	347.589±30.441	-670.765±58.833
DI-GAT	10.106±0.961	-0.592±0.151	11.260±1.237	-2.044±0.334	122.242±11.986	-3.120±0.403	375.266±18.144	-724.255±35.066
BI-GAT	5.699±1.155	0.101±0.181	2.683±0.927	0.274±0.250	78.499±6.022	-1.645±0.202	463.886±29.786	-895.527±57.565
GPS-P	7.241±0.520	-0.140±0.082	5.487±1.351	-0.483±0.365	124.375±114.416	-3.191±3.856	82.559±46.320	-158.557±89.522
DI-GPS-P	6.847±0.879	-0.078±0.138	6.704±5.834	-0.812±1.577	412.567±168.322	-12.905±5.673	72.483±66.727	-139.085±128.960
BI-GPS-P	7.284±0.676	-0.147±0.106	4.192±1.854	-0.133±0.428	69.680±21.461	-1.348±0.723	572.724±92.117	-1105.870±178.030
DGCN	13.362±0.281	-1.105±0.044	13.303±0.332	-2.597±0.089	66.196±22.392	-1.231±0.754	539.409±140.777	-1041.484±272.073
DiGCN	11.603±1.166	-0.828±0.183	10.983±1.244	-1.969±0.336	250.774±175.035	-7.452±5.899	889.065±290.158	-1717.245±560.771
MagNet	8.757±1.044	-0.379±0.164	5.321±1.637	-0.439±0.442	93.389±2.734	-2.147±0.092	425.460±18.451	-821.263±35.659
Timer-inspired GNN	-	0.9135	-	0.8656	-	-	-	-

Table 21: OOD performance on the TIME dataset.

Method	densenets	mnasnets	mobilenetv2s	mobilenetv3s	nasbench201s	average
GCN	43.042±1.663	7.764±0.775	30.222±0.817	5.981±1.454	2.134±0.772	17.828±0.802
DI-GCN	41.241±0.336	6.704±0.183	29.457±0.389	5.275±0.262	1.129±0.426	16.761±0.151
BI-GCN	41.271±1.729	8.054±0.399	29.473±0.399	5.365±0.159	2.114±0.731	17.256±0.238
GIN	7.694±0.442	1.833±0.187	3.535±0.343	1.491±0.343	0.617±0.216	3.034±0.172
DI-GIN	9.894±0.450	1.943±0.116	3.395±0.293	1.157±0.118	0.748±0.118	3.427±0.129
BI-GIN	7.615±0.247	1.901±0.151	3.339±0.172	1.177±0.160	0.493±0.069	2.905±0.098
GAT	14.272±4.836	4.160±0.460	8.733±0.936	3.227±0.456	0.577±0.071	6.194±1.242
DI-GAT	21.741±2.897	3.850±0.418	11.801±1.780	3.640±0.582	1.820±0.159	8.571±0.900
BI-GAT	9.322±0.535	2.371±0.469	4.957±0.497	1.723±0.481	0.498±0.086	3.774±0.262
GPS-P	7.080±0.302	2.125±0.294	3.951±0.289	1.692±0.395	0.723±0.197	3.114±0.132
DI-GPS-P	6.821±0.223	2.016±0.226	3.265±0.494	1.337±0.618	0.620±0.372	2.812±0.257
BI-GPS-P	6.863±0.265	1.971±0.222	3.794±0.311	1.399±0.361	0.618±0.260	2.929±0.149
DGCN	41.386±0.878	6.651±0.253	30.312±0.307	4.591±0.310	2.101±0.211	17.008±0.152
DiGCN	42.506±0.745	7.203±0.137	30.941±0.426	5.263±0.468	1.879±0.558	17.558±0.169
MagNet	7.368±0.189	1.910±0.152	3.015±0.280	1.290±0.315	0.514±0.166	2.819±0.177
nn-meter	7.1	3.19	3.25	2.03	0.44	3.20

Table 22: ID performance on the CG dataset on device ‘Cortex A76 CPU’ with ‘rmse’ metric.

Method	densenets	mnasnets	mobilenetv3s	mobilenetv4s	nasbench202s	average
GCN	0.217±0.034	0.267±0.033	0.118±0.026	0.239±0.090	0.290±0.183	0.226±0.037
DI-GCN	0.222±0.010	0.289±0.022	0.101±0.014	0.264±0.023	0.530±0.184	0.281±0.037
BI-GCN	0.245±0.038	0.269±0.012	0.111±0.022	0.287±0.010	0.272±0.152	0.236±0.031
GIN	0.876±0.028	0.863±0.054	0.680±0.050	0.723±0.078	0.716±0.190	0.771±0.052
DI-GIN	0.764±0.025	0.835±0.040	0.693±0.050	0.805±0.060	0.626±0.114	0.744±0.021
BI-GIN	0.892±0.020	0.842±0.047	0.681±0.033	0.861±0.053	0.858±0.059	0.826±0.024
GAT	0.662±0.107	0.456±0.067	0.359±0.032	0.476±0.060	0.786±0.056	0.547±0.050
DI-GAT	0.466±0.053	0.540±0.062	0.273±0.046	0.375±0.046	0.343±0.077	0.399±0.029
BI-GAT	0.808±0.034	0.746±0.077	0.511±0.065	0.689±0.116	0.844±0.091	0.719±0.051
GPS-P	0.904±0.019	0.809±0.051	0.650±0.041	0.666±0.126	0.697±0.173	0.745±0.057
DI-GPS-P	0.933±0.018	0.831±0.071	0.735±0.038	0.796±0.234	0.750±0.271	0.808±0.104
BI-GPS-P	0.922±0.020	0.836±0.048	0.666±0.051	0.738±0.141	0.750±0.215	0.782±0.072
DGCN	0.188±0.017	0.320±0.019	0.105±0.022	0.294±0.042	0.269±0.042	0.235±0.009
DiGCN	0.199±0.025	0.289±0.035	0.085±0.014	0.288±0.042	0.309±0.111	0.233±0.017
MagNet	0.896±0.012	0.835±0.060	0.730±0.048	0.830±0.113	0.851±0.108	0.828±0.062
nn-meter	0.931	0.824	0.676	0.738	0.824	0.798

Table 23: ID performance on the CG dataset on device ‘Cortex A76 CPU’ with ‘acc5’ metric.

Method	densenets	mnasnets	mobilenetv4s	mobilenetv5s	nasbench203s	average
GCN	0.434±0.041	0.511±0.042	0.222±0.031	0.453±0.122	0.515±0.233	0.426±0.053
DI-GCN	0.446±0.023	0.571±0.023	0.193±0.021	0.476±0.032	0.818±0.158	0.501±0.031
BI-GCN	0.481±0.025	0.483±0.026	0.243±0.018	0.536±0.029	0.517±0.199	0.451±0.037
GIN	0.998±0.004	0.997±0.004	0.936±0.024	0.941±0.044	0.972±0.035	0.968±0.016
DI-GIN	0.984±0.013	0.999±0.003	0.965±0.019	0.982±0.018	0.956±0.025	0.977±0.008
BI-GIN	1.000±0.000	0.996±0.005	0.952±0.018	0.991±0.017	0.994±0.012	0.986±0.007
GAT	0.924±0.091	0.808±0.039	0.645±0.063	0.730±0.060	0.973±0.017	0.816±0.036
DI-GAT	0.757±0.055	0.828±0.054	0.532±0.050	0.650±0.075	0.625±0.071	0.678±0.036
BI-GAT	0.993±0.009	0.977±0.034	0.821±0.057	0.937±0.081	0.994±0.007	0.944±0.026
GPS-P	1.000±0.000	0.996±0.006	0.918±0.033	0.901±0.080	0.928±0.085	0.949±0.034
DI-GPS-P	0.999±0.003	0.997±0.004	0.974±0.018	0.949±0.117	0.940±0.154	0.971±0.055
BI-GPS-P	0.999±0.003	0.998±0.004	0.938±0.021	0.922±0.085	0.953±0.078	0.962±0.030
DGCN	0.409±0.015	0.568±0.021	0.204±0.020	0.538±0.027	0.504±0.076	0.444±0.010
DiGCN	0.390±0.017	0.543±0.017	0.186±0.022	0.522±0.044	0.582±0.156	0.444±0.029
MagNet	1.000±0.000	0.996±0.005	0.973±0.028	0.983±0.031	0.988±0.019	0.988±0.015
nn-meter	0.999	0.992	0.977	0.990	0.999	0.991

Table 24: ID performance on the CG dataset on device ‘Cortex A76 CPU’ with ‘acc10’ metric.

Method	proxylessnass			resnets		
	rmse	acc5	acc10	rmse	acc5	acc10
GCN	38.016±9.318	0.130±0.018	0.237±0.040	529.239±19.212	0.012±0.007	0.017±0.009
DI-GCN	33.581±1.016	0.143±0.019	0.264±0.016	517.553±4.419	0.010±0.002	0.020±0.003
BI-GCN	38.612±2.911	0.112±0.010	0.224±0.007	524.188±11.204	0.008±0.009	0.016±0.011
GIN	18.768±4.710	0.156±0.069	0.333±0.123	326.443±37.550	0.059±0.024	0.112±0.038
DI-GIN	10.742±0.876	0.306±0.021	0.566±0.051	455.235±16.044	0.032±0.010	0.073±0.012
BI-GIN	11.097±2.002	0.329±0.061	0.589±0.096	362.930±29.676	0.046±0.015	0.087±0.013
GAT	20.289±4.934	0.208±0.059	0.396±0.090	467.151±29.254	0.012±0.017	0.025±0.026
DI-GAT	19.306±3.641	0.192±0.043	0.386±0.063	386.181±44.349	0.033±0.023	0.069±0.030
BI-GAT	14.833±4.066	0.237±0.070	0.471±0.132	472.310±24.953	0.019±0.011	0.036±0.014
GPS-P	11.952±2.043	0.275±0.078	0.527±0.104	473.207±15.942	0.013±0.007	0.023±0.011
DI-GPS-P	10.122±0.911	0.293±0.038	0.588±0.075	490.252±11.336	0.005±0.005	0.012±0.009
BI-GPS-P	12.188±1.565	0.249±0.054	0.506±0.074	475.745±14.259	0.005±0.009	0.015±0.012
DGCN	28.038±1.707	0.123±0.016	0.274±0.015	535.961±5.274	0.003±0.005	0.007±0.007
DiGCN	26.308±1.739	0.138±0.017	0.287±0.022	542.416±5.718	0.001±0.002	0.005±0.004
MagNet	9.282±1.321	0.433±0.069	0.725±0.055	483.296±9.749	0.015±0.010	0.024±0.017
nn-meter	3.18	0.846	1.00	7.19	0.845	0.999

Table 25: OOD performance on the CG dataset on device ‘Cortex A76 CPU’.

Method	densenets	mnasnets	mobilenetv3s	mobilenetv4s	nasbench202s	average
GCN	6.330±0.099	1.192±0.035	5.075±0.054	0.811±0.034	0.110±0.029	2.704±0.016
DI-GCN	6.226±0.061	1.165±0.029	5.088±0.035	0.795±0.032	0.128±0.036	2.681±0.013
BI-GCN	6.233±0.140	1.173±0.094	4.091±0.158	0.867±0.098	0.411±0.118	2.555±0.052
GIN	0.514±0.056	0.133±0.021	0.322±0.064	0.110±0.017	0.079±0.020	0.231±0.025
DI-GIN	0.909±0.064	0.176±0.017	0.385±0.036	0.156±0.029	0.250±0.022	0.375±0.019
BI-GIN	0.554±0.038	0.158±0.016	0.357±0.037	0.142±0.021	0.116±0.033	0.265±0.013
GAT	1.742±0.302	0.446±0.079	1.329±0.245	0.349±0.081	0.132±0.050	0.800±0.102
DI-GAT	1.904±0.173	0.531±0.087	1.810±0.414	0.481±0.068	0.497±0.022	1.044±0.133
BI-GAT	0.854±0.057	0.192±0.048	0.510±0.094	0.169±0.035	0.080±0.020	0.361±0.039
GPS-P	0.313±0.021	0.131±0.015	0.286±0.035	0.104±0.013	0.069±0.025	0.181±0.009
DI-GPS-P	0.320±0.020	0.149±0.019	0.321±0.081	0.147±0.029	0.186±0.134	0.225±0.032
BI-GPS-P	0.486±0.062	0.197±0.039	0.508±0.117	0.174±0.047	0.124±0.072	0.298±0.054
DGCN	6.695±0.428	1.267±0.101	5.396±0.050	0.817±0.200	0.614±0.079	2.958±0.074
DiiGCN	6.298±0.165	1.344±0.106	5.508±0.185	0.919±0.107	0.549±0.174	2.924±0.083
MagNet	0.478±0.032	0.120±0.015	0.230±0.017	0.106±0.008	0.060±0.008	0.199±0.008

Table 26: ID performance on the CG dataset on device ‘Adreno 630 GPU’ with ‘rmse’ metric.

Method	densenets	mnasnets	mobilenetv3s	mobilenetv4s	nasbench202s	average
GCN	0.325±0.032	0.383±0.019	0.119±0.015	0.410±0.035	0.943±0.052	0.435±0.013
DI-GCN	0.351±0.014	0.404±0.023	0.127±0.031	0.442±0.047	0.910±0.076	0.447±0.020
BI-GCN	0.354±0.030	0.410±0.040	0.164±0.031	0.424±0.038	0.485±0.100	0.367±0.028
GIN	1.000±0.000	1.000±0.000	0.956±0.032	1.000±0.000	0.994±0.009	0.990±0.007
DI-GIN	0.986±0.014	1.000±0.000	0.916±0.023	0.997±0.006	0.703±0.062	0.920±0.009
BI-GIN	1.000±0.000	1.000±0.000	0.917±0.016	0.991±0.012	0.945±0.057	0.970±0.012
GAT	0.872±0.054	0.864±0.068	0.515±0.070	0.862±0.065	0.907±0.131	0.804±0.050
DI-GAT	0.839±0.049	0.790±0.073	0.344±0.085	0.768±0.047	0.466±0.052	0.641±0.046
BI-GAT	0.989±0.005	0.992±0.013	0.829±0.049	0.993±0.012	0.994±0.009	0.959±0.011
GPS-P	1.000±0.000	1.000±0.000	0.966±0.021	1.000±0.000	0.994±0.015	0.992±0.005
DI-GPS-P	1.000±0.000	1.000±0.000	0.927±0.064	0.976±0.049	0.749±0.351	0.930±0.068
BI-GPS-P	1.000±0.000	0.995±0.005	0.861±0.043	0.972±0.043	0.892±0.156	0.944±0.045
DGCN	0.290±0.019	0.403±0.037	0.114±0.020	0.471±0.113	0.302±0.074	0.316±0.038
DiiGCN	0.302±0.028	0.432±0.042	0.118±0.022	0.441±0.054	0.363±0.146	0.331±0.031
MagNet	1.000±0.000	1.000±0.000	0.978±0.011	1.000±0.000	0.999±0.003	0.995±0.002

Table 27: ID performance on the CG dataset on device ‘Adreno 630 GPU’ with ‘acc5’ metric.

Method	densenets	mnasnets	mobilenetv3s	mobilenetv4s	nasbench202s	average
GCN	0.608±0.017	0.716±0.022	0.227±0.018	0.780±0.048	0.998±0.004	0.665±0.009
DI-GCN	0.614±0.014	0.741±0.021	0.225±0.015	0.792±0.048	0.992±0.013	0.672±0.013
BI-GCN	0.629±0.028	0.772±0.048	0.312±0.029	0.747±0.086	0.789±0.088	0.650±0.037
GIN	1.000±0.000	1.000±0.000	0.994±0.007	1.000±0.000	1.000±0.000	0.999±0.001
DI-GIN	1.000±0.000	1.000±0.000	0.994±0.005	1.000±0.000	0.904±0.010	0.979±0.002
BI-GIN	1.000±0.000	1.000±0.000	0.993±0.006	1.000±0.000	0.980±0.024	0.994±0.004
GAT	0.989±0.017	0.992±0.013	0.802±0.079	0.989±0.018	0.993±0.018	0.953±0.024
DI-GAT	0.991±0.005	0.980±0.020	0.630±0.106	0.962±0.014	0.715±0.033	0.855±0.029
BI-GAT	1.000±0.000	1.000±0.000	0.985±0.012	1.000±0.000	1.000±0.000	0.997±0.002
GPS-P	1.000±0.000	1.000±0.000	0.998±0.006	1.000±0.000	1.000±0.000	0.999±0.001
DI-GPS-P	1.000±0.000	1.000±0.000	0.988±0.021	1.000±0.000	0.947±0.157	0.986±0.030
BI-GPS-P	1.000±0.000	1.000±0.000	0.990±0.010	0.998±0.003	0.961±0.059	0.990±0.012
DGCN	0.564±0.022	0.708±0.031	0.200±0.016	0.781±0.103	0.611±0.099	0.573±0.041
DiiGCN	0.597±0.017	0.721±0.031	0.220±0.033	0.724±0.088	0.613±0.197	0.575±0.054
MagNet	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000

Table 28: ID performance on the CG dataset on device ‘Adreno 630 GPU’ with ‘acc10’ metric.

Method	proxylessnass			resnets		
	rmse	acc5	acc10	rmse	acc5	acc10
GCN	6.517±0.386	0.150±0.019	0.275±0.017	111.019±1.367	0.006±0.005	0.015±0.007
DI-GCN	6.135±0.149	0.154±0.021	0.305±0.014	111.631±1.095	0.007±0.005	0.012±0.006
BI-GCN	5.314±0.297	0.150±0.013	0.294±0.023	98.142±2.642	0.002±0.004	0.006±0.003
GIN	3.252±0.272	0.279±0.046	0.512±0.024	90.353±5.675	0.030±0.012	0.066±0.017
DI-GIN	3.121±0.549	0.271±0.076	0.514±0.079	109.263±2.076	0.028±0.013	0.057±0.011
BI-GIN	3.307±0.184	0.306±0.044	0.538±0.020	99.362±2.257	0.030±0.017	0.053±0.020
GAT	3.082±0.419	0.252±0.065	0.479±0.084	95.114±5.394	0.011±0.014	0.025±0.030
DI-GAT	3.982±0.341	0.172±0.019	0.355±0.027	92.212±9.020	0.035±0.019	0.072±0.029
BI-GAT	3.461±0.376	0.265±0.038	0.476±0.059	109.787±1.405	0.003±0.005	0.005±0.009
GPS-P	2.554±0.146	0.304±0.068	0.639±0.022	104.410±1.863	0.010±0.005	0.019±0.006
DI-GPS-P	2.515±0.148	0.270±0.070	0.614±0.061	105.275±2.238	0.006±0.010	0.009±0.013
BI-GPS-P	2.793±0.261	0.281±0.064	0.542±0.091	104.383±3.367	0.009±0.007	0.018±0.011
DGCN	5.794±0.249	0.160±0.012	0.293±0.026	116.229±1.179	0.006±0.006	0.017±0.010
DiGCN	6.042±0.906	0.140±0.023	0.271±0.043	117.250±1.149	0.006±0.005	0.013±0.008
MagNet	3.120±0.409	0.434±0.077	0.599±0.070	109.707±2.288	0.001±0.002	0.003±0.003

Table 29: OOD performance on the CG dataset on device ‘Adreno 630 GPU’.

Method	densenets	mnasnets	mobilenetv3s	mobilenetv4s	nasbench202s	average
GCN	4.754±0.087	1.141±0.032	4.717±0.039	0.820±0.042	0.184±0.075	2.323±0.026
DI-GCN	4.899±0.188	1.159±0.064	4.869±0.179	0.834±0.070	0.162±0.102	2.385±0.084
BI-GCN	4.712±0.095	1.150±0.061	3.834±0.104	0.887±0.142	0.364±0.116	2.190±0.042
GIN	0.847±0.089	0.249±0.176	0.518±0.161	0.216±0.076	0.539±0.511	0.474±0.103
DI-GIN	0.639±0.034	0.119±0.013	0.303±0.019	0.102±0.023	0.050±0.010	0.243±0.011
BI-GIN	0.310±0.022	0.100±0.011	0.231±0.015	0.099±0.028	0.039±0.013	0.156±0.011
GAT	1.630±0.299	0.441±0.088	1.585±0.311	0.388±0.052	0.131±0.081	0.835±0.127
DI-GAT	1.763±0.174	0.576±0.097	1.589±0.162	0.513±0.087	0.429±0.049	0.974±0.077
BI-GAT	0.830±0.082	0.269±0.026	0.834±0.114	0.264±0.030	0.062±0.020	0.452±0.032
GPS-P	0.303±0.035	0.132±0.020	0.335±0.043	0.112±0.026	0.106±0.062	0.197±0.015
DI-GPS-P	0.316±0.030	0.145±0.020	0.332±0.042	0.110±0.009	0.060±0.032	0.193±0.018
BI-GPS-P	0.296±0.012	0.118±0.016	0.303±0.049	0.083±0.011	0.108±0.071	0.182±0.026
DGCN	4.903±0.105	1.162±0.047	5.048±0.030	0.756±0.060	0.409±0.045	2.456±0.032
DiiGCN	4.807±0.174	1.274±0.118	5.139±0.174	0.834±0.091	0.470±0.075	2.505±0.094
MagNet	0.583±0.051	0.155±0.019	0.337±0.042	0.150±0.029	0.074±0.031	0.260±0.019

Table 30: ID performance on the CG dataset on device ‘Adreno 640 GPU’ with ‘rmse’ metric.

Method	densenets	mnasnets	mobilenetv3s	mobilenetv4s	nasbench202s	average
GCN	0.367±0.014	0.381±0.024	0.133±0.020	0.422±0.034	0.678±0.320	0.396±0.066
DI-GCN	0.357±0.016	0.416±0.035	0.139±0.029	0.450±0.047	0.782±0.272	0.429±0.059
BI-GCN	0.412±0.040	0.447±0.038	0.178±0.024	0.422±0.084	0.383±0.180	0.368±0.050
GIN	0.986±0.009	0.951±0.124	0.806±0.103	0.943±0.081	0.515±0.409	0.840±0.095
DI-GIN	0.999±0.003	1.000±0.000	0.962±0.023	1.000±0.000	0.997±0.006	0.991±0.004
BI-GIN	1.000±0.000	1.000±0.000	0.983±0.006	0.999±0.003	1.000±0.000	0.996±0.001
GAT	0.846±0.057	0.861±0.075	0.427±0.064	0.821±0.069	0.830±0.287	0.757±0.078
DI-GAT	0.836±0.042	0.744±0.080	0.373±0.053	0.674±0.101	0.424±0.058	0.610±0.047
BI-GAT	0.990±0.006	0.981±0.015	0.671±0.047	0.926±0.038	0.989±0.009	0.911±0.014
GPS-P	1.000±0.000	1.000±0.000	0.938±0.038	1.000±0.000	0.890±0.234	0.965±0.049
DI-GPS-P	1.000±0.000	1.000±0.000	0.950±0.032	0.998±0.006	0.994±0.018	0.988±0.009
BI-GPS-P	1.000±0.000	1.000±0.000	0.960±0.043	1.000±0.000	0.876±0.196	0.967±0.047
DGCN	0.343±0.020	0.409±0.028	0.122±0.022	0.510±0.077	0.441±0.088	0.365±0.017
DiiGCN	0.343±0.031	0.415±0.036	0.116±0.017	0.456±0.080	0.383±0.092	0.342±0.028
MagNet	0.999±0.003	0.999±0.003	0.922±0.028	0.990±0.014	0.966±0.054	0.975±0.016

Table 31: ID performance on the CG dataset on device ‘Adreno 640 GPU’ with ‘acc5’ metric.

Method	densenets	mnasnets	mobilenetv3s	mobilenetv4s	nasbench202s	average
GCN	0.694±0.011	0.747±0.018	0.249±0.013	0.768±0.061	0.957±0.090	0.683±0.024
DI-GCN	0.684±0.027	0.717±0.023	0.257±0.037	0.728±0.068	0.941±0.128	0.665±0.032
BI-GCN	0.704±0.022	0.757±0.047	0.346±0.031	0.715±0.107	0.712±0.178	0.646±0.054
GIN	1.000±0.000	1.000±0.000	0.959±0.048	0.997±0.006	0.635±0.396	0.918±0.076
DI-GIN	1.000±0.000	1.000±0.000	0.999±0.003	1.000±0.000	1.000±0.000	0.999±0.000
BI-GIN	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000
GAT	0.992±0.010	0.991±0.014	0.701±0.104	0.985±0.009	0.985±0.038	0.930±0.026
DI-GAT	0.984±0.015	0.956±0.032	0.669±0.051	0.949±0.043	0.675±0.055	0.846±0.028
BI-GAT	1.000±0.000	1.000±0.000	0.926±0.020	0.999±0.003	1.000±0.000	0.985±0.004
GPS-P	1.000±0.000	1.000±0.000	0.998±0.004	1.000±0.000	0.990±0.022	0.997±0.005
DI-GPS-P	1.000±0.000	1.000±0.000	0.999±0.003	1.000±0.000	1.000±0.000	0.999±0.000
BI-GPS-P	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	0.986±0.023	0.997±0.004
DGCN	0.664±0.024	0.722±0.024	0.231±0.022	0.800±0.061	0.699±0.082	0.623±0.026
DiiGCN	0.662±0.031	0.703±0.027	0.218±0.030	0.745±0.067	0.617±0.114	0.589±0.031
MagNet	1.000±0.000	1.000±0.000	0.994±0.007	1.000±0.000	0.999±0.003	0.998±0.001

Table 32: ID performance on the CG dataset on device ‘Adreno 640 GPU’ with ‘acc10’ metric.

Method	proxylssnass			resnets		
	rmse	acc5	acc10	rmse	acc5	acc10
GCN	5.600±0.162	0.169±0.018	0.303±0.018	82.509±1.149	0.006±0.004	0.011±0.004
DI-GCN	6.163±0.463	0.145±0.013	0.283±0.022	82.785±1.409	0.007±0.004	0.015±0.004
BI-GCN	5.039±0.203	0.147±0.012	0.279±0.021	70.904±1.024	0.001±0.002	0.003±0.004
GIN	3.704±0.383	0.267±0.057	0.488±0.069	65.961±7.773	0.029±0.014	0.067±0.027
DI-GIN	3.672±0.328	0.249±0.028	0.461±0.044	62.820±4.603	0.038±0.008	0.078±0.017
BI-GIN	3.326±0.218	0.285±0.031	0.535±0.042	69.651±5.469	0.037±0.010	0.067±0.016
GAT	3.646±0.751	0.212±0.058	0.408±0.089	66.092±7.723	0.018±0.012	0.039±0.029
DI-GAT	4.893±0.580	0.155±0.031	0.312±0.048	69.358±4.897	0.022±0.012	0.047±0.022
BI-GAT	3.666±0.544	0.246±0.057	0.453±0.080	76.832±4.857	0.000±0.001	0.001±0.003
GPS-P	2.789±0.093	0.293±0.086	0.627±0.021	74.002±1.594	0.006±0.005	0.011±0.006
DI-GPS-P	2.883±0.134	0.303±0.053	0.605±0.038	76.163±2.222	0.006±0.004	0.016±0.011
BI-GPS-P	2.747±0.101	0.283±0.063	0.653±0.020	72.210±0.404	0.011±0.002	0.020±0.005
DGCN	4.985±0.157	0.160±0.016	0.300±0.018	85.713±1.394	0.007±0.007	0.011±0.009
DiiGCN	5.362±0.645	0.148±0.012	0.299±0.020	86.605±0.664	0.003±0.003	0.004±0.005
MagNet	3.309±0.187	0.431±0.030	0.594±0.043	77.379±1.987	0.004±0.006	0.005±0.008

Table 33: OOD performance on the CG dataset on device ‘Adreno 640 GPU’.

H.2 COMPARISON BETWEEN NPE AND EPE

Method	gain		PM		BW	
	mse	rmse	mse	rmse	mse	rmse
BI-GIN+NPE	0.135±0.009	0.367±0.012	1.296±0.024	1.138±0.010	19.215±1.044	4.382±0.117
BI-GINE+EPE	0.149±0.009	0.386±0.012	1.283±0.033	1.132±0.014	17.399±0.644	4.170±0.076
BI-GPS+NPE	0.122±0.007	0.349±0.010	1.212±0.058	1.100±0.026	20.475±8.853	4.456±0.825
BI-GPS+EPE	0.115±0.008	0.339±0.011	1.206±0.090	1.097±0.040	18.153±2.235	4.253±0.256

Table 34: NPE v.s. EPE on ID data on the AMP dataset.

method	dsp		lut		cp	
	mse	r2	mse	r2	mse	r2
BI-GINE+NPE	2.508±0.183	0.977±0.001	1.983±0.078	0.879±0.006	0.617±0.026	0.858±0.004
BI-GINE+EPE	2.127±0.085	0.981±0.000	1.729±0.096	0.895±0.007	0.607±0.022	0.857±0.007
BI-GPS+NPE	2.442±0.303	0.979±0.002	2.112±0.216	0.873±0.014	0.621±0.018	0.859±0.009
BI-GPS+EPE	2.133±0.148	0.981±0.001	1.957±0.125	0.883±0.011	0.602±0.017	0.861±0.007

Table 35: NPE v.s. EPE on ID data on the HLS dataset.

	shared				root			
	accuracy	precision	recall	f1	accuracy	precision	recall	f1
BI-GIN+NPE	0.999±0.000	0.987±0.039	0.999±0.000	0.991±0.026	0.999±0.000	0.999±0.000	0.999±0.000	0.999±0.000
BI-GIN+EPE	0.999±0.001	0.974±0.079	0.974±0.078	0.974±0.079	0.999±0.000	0.999±0.000	0.999±0.000	0.999±0.000

Table 36: NPE v.s. EPE on ID data on the SR dataset.

	method	blabla	usb_cdc_core	wbqspiflash	cic_decimator	picorv32a	zipdiv	usb	average
hold rmse	BI-GINE+NPE	0.449±0.106	0.327±0.161	0.162±0.051	0.063±0.025	2.006±0.115	0.107±0.080	0.049±0.018	0.452±0.040
	BI-GINE+EPE	0.181±0.059	0.021±0.008	0.031±0.006	0.010±0.003	0.652±0.070	0.026±0.011	0.014±0.002	0.134±0.012
hold R2	BI-GINE+NPE	0.995±0.001	0.834±0.081	0.940±0.018	0.928±0.028	0.855±0.008	0.970±0.022	0.928±0.026	0.921±0.018
	BI-GINE+EPE	0.998±0.000	0.988±0.004	0.981±0.003	0.993±0.002	0.954±0.004	0.993±0.002	0.986±0.002	0.985±0.001
setup rmse	BI-GINE+NPE	55.889±2.928	5.481±1.416	13.006±2.716	2.438±0.606	34.429±2.865	12.805±4.583	1.728±0.331	17.968±1.206
	BI-GINE+EPE	15.134±2.195	1.327±0.747	2.718±1.297	0.966±0.877	17.996±3.227	6.436±5.416	0.885±0.317	6.494±1.449
setup R2	BI-GINE+NPE	0.142±0.044	-0.021±0.264	0.326±0.140	-0.149±0.285	0.173±0.068	0.364±0.227	0.306±0.132	0.163±0.093
	BI-GINE+EPE	0.767±0.033	0.752±0.139	0.859±0.067	0.544±0.413	0.567±0.077	0.680±0.268	0.644±0.127	0.688±0.091

Table 37: NPE v.s. EPE on ID data on the TIME dataset.

	Method	densenets	mnasnets	mobilenetv2s	mobilenetv3s	nasbench201s	average
cpu rmse	BI-GIN+NPE	7.734±0.602	2.053±0.235	3.788±0.424	1.590±0.371	0.725±0.173	3.178±0.168
	BIGINE+EPE	7.550±0.291	1.728±0.224	3.064±0.326	1.176±0.155	0.419±0.033	2.788±0.147
cpu acc5	BI-GIN+NPE	0.893±0.014	0.821±0.056	0.653±0.052	0.705±0.153	0.545±0.351	0.723±0.104
	BIGINE+EPE	0.907±0.017	0.873±0.042	0.766±0.041	0.861±0.036	0.901±0.029	0.861±0.019
cpu acc10	BI-GIN+NPE	0.999±0.003	0.994±0.006	0.940±0.025	0.907±0.066	0.940±0.060	0.956±0.028
	BIGINE+EPE	1.000±0.000	0.999±0.003	0.969±0.023	0.994±0.009	0.999±0.003	0.992±0.006
gpu630 rmse	BI-GIN+NPE	0.440±0.020	0.112±0.009	0.254±0.019	0.099±0.014	0.056±0.006	0.192±0.006
	BIGINE+EPE	0.293±0.024	0.109±0.020	0.272±0.035	0.092±0.021	0.073±0.027	0.168±0.009
gpu630 acc5	BI-GIN+NPE	1.000±0.000	1.000±0.000	0.974±0.015	1.000±0.000	1.000±0.000	0.994±0.003
	BIGINE+EPE	1.000±0.000	1.000±0.000	0.968±0.026	1.000±0.000	0.978±0.052	0.989±0.010
gpu630 acc10	BI-GIN+NPE	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000
	BIGINE+EPE	1.000±0.000	1.000±0.000	0.999±0.003	1.000±0.000	1.000±0.000	0.999±0.000
gpu640 rmse	BI-GIN+NPE	0.355±0.031	0.146±0.017	0.289±0.024	0.157±0.031	0.071±0.018	0.204±0.009
	BIGINE+EPE	0.343±0.028	0.089±0.011	0.245±0.027	0.093±0.016	0.046±0.018	0.163±0.010
gpu640 acc5	BI-GIN+NPE	1.000±0.000	1.000±0.000	0.971±0.015	0.949±0.081	0.986±0.012	0.981±0.016
	BIGINE+EPE	1.000±0.000	1.000±0.000	0.987±0.013	1.000±0.000	1.000±0.000	0.997±0.002
gpu640 acc10	BI-GIN+NPE	1.000±0.000	1.000±0.000	0.996±0.005	1.000±0.000	0.999±0.003	0.999±0.001
	BIGINE+EPE	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000	1.000±0.000

Table 38: NPE v.s. EPE on ID data on the CG dataset.

Method	gain		PM		BW	
	mse	rmse	mse	rmse	mse	rmse
BI-GIN+NPE	0.303±0.046	0.549±0.042	1.379±0.027	1.174±0.011	25.967±1.646	5.093±0.161
BI-GINE+EPE	0.302±0.037	0.549±0.033	1.373±0.005	1.171±0.002	22.339±1.413	4.724±0.150
BI-GPS+NPE	0.314±0.030	0.560±0.027	1.315±0.050	1.146±0.021	26.607±10.277	5.087±0.897
BI-GPS+EPE	0.302±0.071	0.546±0.060	1.314±0.143	1.126±0.060	21.815±1.973	4.666±0.206

Table 39: NPE v.s. EPE on OOD data on the AMP dataset.

method	dsp		lut		cp	
	mse	r2	mse	r2	mse	r2
BI-GINE+NPE	3.434±0.238	0.964±0.002	0.113±0.019	0.971±0.004	0.450±0.013	0.830±0.008
BI-GINE+EPE	3.243±0.098	0.966±0.000	0.102±0.019	0.973±0.005	0.452±0.022	0.823±0.011
BI-GPS+NPE	3.209±0.263	0.967±0.001	0.133±0.027	0.968±0.006	0.496±0.017	0.812±0.016
BI-GPS+EPE	3.205±0.026	0.968±0.001	0.102±0.017	0.972±0.003	0.474±0.017	0.830±0.006

Table 40: NPE v.s. EPE on OOD data on the HLS dataset.

	shared				root			
	accuracy	precision	recall	f1	accuracy	precision	recall	f1
BI-GIN+NPE	0.712±0.027	0.510±0.103	0.591±0.021	0.502±0.032	0.696±0.057	0.556±0.066	0.616±0.072	0.567±0.068
BI-GINE+EPE	0.725±0.037	0.510±0.059	0.604±0.030	0.530±0.038	0.747±0.035	0.569±0.113	0.508±0.080	0.520±0.090

Table 41: NPE v.s. EPE on OOD data on the SR dataset.

	Method	xtea		synth_ram	
		mse	r2	mse	r2
hold	BI-GINE+NPE	6.936±0.914	-0.092±0.144	0.743±0.313	0.798±0.084
	BI-GINE+-EPE	2.074±0.474	0.673±0.074	0.617±0.906	0.832±0.245
setup	BI-GINE+NPE	98.690±55.964	-2.326±1.886	629.630±107.437	-1215.849±207.638
	BI-GINE+-EPE	59.401±13.573	-1.002±0.457	619.030±136.176	-1195.363±263.179

Table 42: NPE v.s. EPE on OOD data on the TIME dataset.

	Method	proxylessnas			resnets		
		rmse	acc5	acc10	rmse	acc5	acc10
cpu	BI-GIN+NPE	15.045±5.642	0.264±0.138	0.487±0.199	388.079±36.250	0.041±0.014	0.073±0.024
	BI-GINE+EPE	11.049±0.909	0.310±0.024	0.588±0.049	381.432±28.102	0.036±0.009	0.072±0.016
gpu630	BI-GIN+NPE	2.843±0.289	0.277±0.031	0.538±0.055	97.056±7.138	0.034±0.012	0.065±0.020
	BI-GINE+EPE	2.947±0.239	0.370±0.082	0.595±0.051	108.959±2.594	0.020±0.011	0.033±0.018
gpu640	BI-GIN+NPE	3.591±0.286	0.303±0.062	0.549±0.050	76.590±4.263	0.024±0.009	0.048±0.011
	BI-GINE+EPE	3.419±0.266	0.295±0.034	0.525±0.050	68.530±3.603	0.037±0.020	0.065±0.023

Table 43: NPE v.s. EPE on OOD data on the CG dataset.