BRP-NAS: Prediction-based NAS using GCNs

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Abstract

Neural architecture search (NAS) enables researchers to automatically explore broad design spaces in order to improve efficiency of neural networks. This efficiency is especially important in the case of on-device deployment, where improvements in accuracy should be balanced out with computational demands of a model. In practice, performance metrics of model are computationally expensive to obtain. Previous work uses a proxy (e.g. number of operations) or a layer-wise measurement of neural network layers to estimate end-to-end hardware performance but the imprecise prediction diminishes the quality of NAS. To address this problem, we propose BRP-NAS, an efficient hardware-aware NAS enabled by an accurate performance predictor-based on graph convolutional network (GCN). What is more, we investigate prediction quality on different metrics and show that sample-efficiency of the predictor-based NAS can be improved by considering binary relations of models and an iterative data selection strategy. We show that our proposed method outperforms all prior methods on both NAS-Bench-101 and NAS-Bench-201. Finally, to raise awareness of the fact that accurate latency estimation is not a trivial task, we release LatBench - a latency dataset of NAS-Bench-201 models running on a broad range of devices.

1 Introduction

Neural architecture search (NAS) has demonstrated great success in automatically designing competitive neural networks compared with hand-crafted alternatives \cite{1 2 3 4}. However, NAS is computationally expensive requiring to train models \cite{5 6} or introduce non-trivial complexity into the search process \cite{7 8}. Additionally, real-world deployment demands models meeting efficiency or hardware constraints (e.g., latency, memory and energy consumption) on top of being accurate, but acquiring various performance metrics of a model can also be time consuming, independently from the cost of training it.

Several works have been proposed to predict performance metrics such as accuracy and latency, the two most popular metrics of interest, instead of measuring them \cite{9 10 11}. Recent work on latency either measures the latency directly from devices during the search process \cite{12 13}, which is accurate but slow and expensive, or rely on a proxy metric (e.g. FLOPS or model size) \cite{14}, which is fast but inaccurate. More recently, layer-wise predictors have been proposed \cite{4} which effectively sum up the latencies of individual neural network layers. While being more accurate than the proxy, layer-wise predictors have a significant drawback: they do not capture the complexities of multiple layer executing on real hardware. In this paper, we (a) show the limitations of the layer-wise predictor both in terms of prediction accuracy and NAS performance and (b) propose a Graph convolutional

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networks (GCN)-based predictor for the end-to-end latency which significantly outperforms the layer-wise approach on devices of various specifications.

Unlike latency prediction, which remains largely unstudied, various end-to-end predictors have been proposed and studied for accuracy. Initially, accuracy predictors were shown to be helpful in guiding a NAS [9]. More recently, it has been shown that accuracy predictor alone can be used to perform a search [10]. One of the key challenges in obtaining a reliable accuracy predictor is the fact that acquiring training samples (pairs of (model, accuracy)) is computationally expensive. Sample efficiency denotes how many samples are required to find the best model during a search under a target hardware constraint, and significantly advancing this metric is a key contribution of our work. We propose several methods to improve sample efficiency – (a) We observe that in the context of NAS, instead of getting a precise estimates of accuracy, we want to produce a linear ordering of accuracy to search for the best model. Therefore, we propose a binary relation predictor to decide the accuracy ranking of neural networks without requiring the predictor to estimate absolute accuracy values. (b) To help the predictor focus on predicting the rankings of top candidates, which is the most important to yield the best results in NAS, we propose an iterative data selection scheme which vastly improves the sample efficiency of NAS.

The contributions of this paper are summarized as follows:

- **Latency prediction.** We empirically show that an accurate latency predictor plays an important role in NAS where latency on the target hardware is of interest, and existing latency predictors are overly error-prone. We propose an end-to-end NAS latency predictor-based on a GCN and show that it outperforms previous approaches (proxy, layer-wise) on various devices. To the best of our knowledge, this is the first end-to-end latency predictor. We illustrate its behaviour on various devices and show that this predictor works well across all of them (Section 3).

- **Accuracy prediction.** We introduce a novel training methodology for a NAS-specific accuracy predictor by turning an accuracy prediction problem into a binary prediction problem, where we predict which one of two neural architectures performs better, resulting in improved overall ranking correlation between predicted and ground-truth rankings. (Section 4).

- **Prediction-based NAS.** We propose a new prediction-based NAS framework called BRP-NAS. It combines a binary relation accuracy predictor architecture and an iterative data selection strategy to improve the top-K ranking correlation. BRP-NAS outperforms previous NAS methods by being up to 3x more sample efficient. Comparing to prior work, our framework is able to find more accurate models more efficiently (Section 4).

- **Towards reproducible research: latency benchmark.** We introduce LatBench, the first large-scale latency measurement dataset for multi-objective NAS. Unlike existing datasets which either approximate the latency or focus on a single device, LatBench provides measurement dataset on a broad range of systems covering desktop CPU/GPU, embedded GPU/TPU and mobile GPU/DSP (Section 5).

2 Related Work

**NAS and performance estimation.** Performance of a neural network is captured by several metrics, such as accuracy, latency, and energy consumption. Because measuring performance metrics is expensive both in terms of time and computation, interest in predicting them has surged since neural architecture search was introduced in [5]. Among several metrics, accuracy prediction is arguably the most actively studied in the context of NAS. Earlier performance prediction works focused on extrapolating the learning curve to reduce the training time [15, 16, 17]. Recent works, on the other hand, explored performance prediction based on architectural properties. For instance, it was demonstrated that an accuracy predictor trained during the search could be successfully used to guide it and, in turn, accelerate it [9]. Taking advantage of the differentiability of accuracy predictors, [18] introduced a gradient-based optimization of neural architectures. Closely related to our work, [10] used graph neural network-based accuracy predictors and an iterative approach to estimate the accuracy of models. However, instead of training the predictor with the top-k mutated models based on previously found models, we trained the predictor by picking both the top-k and random models from the entire search space, an technique that balances exploration and exploitation. Additionally, we
incorporate transfer learning to further boost the performance of the predictor as shown in Section 3.3. Recent focus has been on improving sample efficiency. In that regard, [19] proposed adapting the action space during NAS, where a Monte-Carlo tree search was used to split the action space into good and bad regions. Towards the same goal, [11] introduced a simple NAS based on accuracy predictor, where models with the top-K best predicted accuracy were fully trained, after which the best one was chosen.

**Focused latency prediction.** Latency estimation is of particular importance in hardware-aware NAS. While it is often easier to measure latency than accuracy of a model, measuring latency on general devices (e.g. mobile devices [12]) still takes considerable time when performed for, potentially, thousands of models during NAS. To overcome this challenge, FLOPS and model size have been used as proxies to approximate the overall latency [14]. Additionally, layer-wise approaches [4, 13] are often used to estimate latency of a model as the sum of the latency of each of its operations.

**Multiobjective NAS.** A few works have explored NAS with multiple objectives and hardware constraints. Among those, [20] proposed a hardware-aware adaptation of neural architectures via evolutionary search, where the performance metrics of each architecture were estimated by the predictors. Latency was estimated via a lookup table while accuracy and energy consumption predictors were modeled as Gaussian process regression.

## 3 Latency prediction in NAS

In this section, we demonstrate the limitations of existing latency predictors and introduce a GCN-based latency predictor which (a) significantly outperforms the existing predictors on a wide range of devices in absolute accuracy and (b) contributes to a significant improvement in NAS for latency constrained deployment. Throughout the paper, we focus on NAS-Bench-201 dataset which includes 15,625 models. We use desktop CPU, desktop GPU, embedded GPU and embedded TPU to refer to the devices used in our analysis, with device details described in Section 5.

### 3.1 Existing latency predictors and their limitations in NAS

FLOPS and the number of parameters are often used as proxies for latency estimation for their simplicity but have been shown to be inaccurate in many cases [13, 21]. In Figure 1 (left), we show the scatter plot of models taken from NAS-Bench-201 dataset that illustrates the connection between the latency and FLOPS. Each point in the plots represents the average latency of running a model on the stated device. We can see that latency is not strongly correlated with FLOPS. Recent works [4, 13] use a layer-wise predictor which derives the latency by summing latency measured for each operation in the model individually. However, as shown in Figure 1 (middle), the layer-wise predictor also leads to inaccurate predictions of the end-to-end latency. It assumes sequential processing of operations and cannot reflect the key model and hardware characteristics that affect the end-to-end latency, e.g. whether operations within a model can be executed in parallel on the target hardware, or if execution of an operation is limited due to memory access rather than compute. In section 3.2, we introduce an end-to-end latency predictor that is trained with the end-to-end measured latency that significantly improves the prediction accuracy as shown in Figure 1 (right).

![Figure 1: (Left) FLOPS is not a good proxy for the latency estimation. Our GCN-based end-to-end latency predictor (right) is more accurate than layer-wise predictor (middle). Results shown here are based on desktop CPU.](image)

**NAS with latency predictors.** We analyze the impact of layer-wise latency predictor on NAS for latency-constrained deployment, where the objective is to find the most accurate model that satisfies
a strict latency constraint (e.g. for real-time applications \cite{22,23}). We consider two NAS algorithms, oracle NAS and Aging Evolution \cite{24}. Oracle NAS returns the best accuracy among models such that the latency satisfies the target constraint (more details are provided in the S.M.). In Figure 2 (left), we plot the difference between the best achievable accuracy and the best accuracy obtained by an oracle NAS that relies on the predicted latency - as a function of the target latency constraint. We can see that the accuracy loss due to the inaccurate predictor is non-negligible and sometimes very large (up to 8\%). This loss is also visible when other NAS algorithms are used. In Figure 2 (right), we plot the best accuracy of models found by the aging-evolution search with predicted latency and measured latency as a function of search step. These experimental results highlight the importance of an accurate latency predictor in NAS.

Figure 2: Importance of an accurate latency predictor in NAS for latency-constrained deployment – (Left) Best achievable models missed when using an oracle NAS that relies on predicted latency on desktop GPU. The gap between the layer-wise and GCN curves shows the impact of poor latency predictor. (Right) Best accuracy of models found by the aging-evolution search with predicted latency and measured latency on desktop GPU with 5ms latency limit.

Analysis of Pareto-optimal models. In order to systematically study the impact of inaccurate predictions on latency-aware NAS, we run an analysis of the Pareto-optimal models. Pareto-optimal models are solutions to NAS given a strict latency constraint or if the objective is a weighted combination of the accuracy and the latency \cite{25}. We ask the following: can the Pareto-optimal models be discovered when a latency predictor is used? Suppose we are given an oracle NAS algorithm that returns a Pareto-optimal model based on the accuracy and predicted latency. How far off is that model from the desired Pareto-optimal solution in the accuracy and measured latency plot? In Figure 3 (left and middle), we show scatter plots of NAS-Bench-201 \cite{26} models, where the y-axis represents the accuracy and the x-axis represents latency predicted via the layer-wise predictor (left), and measured latency (middle), respectively. Pareto-optimal models in the predicted space and measured space are marked with pink (o) and red (x), respectively, and shown in both figures. We can see that the Pareto-optimal models in one space do not always lie at the Pareto frontier of the other space. This is problematic because it implies that even if we had a perfect NAS algorithm that discovers Pareto optimal points (based on the predicted latency), there is a high chance that discovered models would not be Pareto optimal in practice.

3.2 End-to-end GCN-based latency predictor.

Our proposed end-to-end latency predictor consists of a GCN which learns models for graph-structure data \cite{27}. Given a graph $g = (V, E)$, where $V$ is a set of $N$ nodes with $D$ features and $E$ is a set of edges, a GCN takes as input a feature description $X \in \mathbb{R}^{N \times D}$ and a description of the graph structure as an adjacency matrix $A \in \mathbb{R}^{N \times N}$. For an $L$-layer GCN, the layer-wise propagation rule is the following:

$$H^{l+1} = f(H^l, A) = \sigma (AH^lW^l),$$

where $H^l$ and $W^l$ are the feature map and weight matrix at the $l$-th layer respectively, and $\sigma(\bullet)$ is a non-linear activation function like ReLU. $H^0 = X$ and $H^L$ is the output with node-level representations.
Figure 3: Red (x), Pink (o), Green marks (*) represent Pareto-optimal models on accuracy vs. measured latency, layer-wise predicted latency, and GCN predicted latency, respectively, on desktop GPU. (Left) Many Pareto-optimal models (red, x) are not located at the Pareto-frontier implying that an oracle NAS cannot discover Pareto-optimal models with the layer-wise predicted latency. (Right) Most Pareto-optimal points (red, x) are located at the Pareto-frontier implying that an oracle NAS is able to discover Pareto-optimal models with our GCN predicted latency.

**Architecture.** Our GCN predictor has 4 layers of GCNs, with 600 hidden units in each layer, followed by a fully connected layer that generates a scalar prediction of the latency. The input neural network model to the GCN is encoded by an adjacency matrix A (asymmetric as the computation flow is represented as a directed graph) and a feature matrix X (one-hot encoding). We also introduce a global node (the node that connects to all the other node) to capture the graph embedding of neural architecture by aggregating all node-level information. GCN can handle any set of neural network models. The details of models used in this paper are in the S.M.

**Training.** All predictors are trained for 100 times, each time using a randomly sampled set of 900 models from the NAS-Bench-201 dataset. 100 random models are used for validation and the remaining 14k models are used for testing.

**Results.** As shown in Figure 1, our GCN predictor outperforms existing predictors, establishing new state-of-the-art, and demonstrates strong performance suitable for NAS (Figure 3). In Table 1, we show the performance of the proposed GCN latency predictor comparing to the layer-wise predictor on various devices. The values are the percentage of models with predicted latency within the corresponding error bound relative to the measured latency. We can see that the strong performance generalizes across various devices, which have vastly different latency behaviors. We provide an extensive study on the latency behavior on various devices in the S.M.

| Error bound | Accuracy of GCN predictor [%] | Accuracy of Layer-wise predictor [%] |
|-------------|-------------------------------|--------------------------------------|
|             | Desktop CPU | Desktop GPU | Embedded GPU | Desktop CPU | Desktop GPU | Embedded GPU |
| ±1%         | 36.0±3.5     | 36.7±4.0     | 24.3±1.4     | 3.5±0.2      | 4.2±0.2      | 6.1±0.3      |
| ±5%         | 85.2±1.8     | 85.9±1.9     | 82.5±1.5     | 18.2±0.4     | 17.1±0.3     | 29.7±0.8     |
| ±10%        | 96.4±0.7     | 96.9±0.8     | 96.3±0.5     | 29.6±1.1     | 32.6±1.2     | 54.0±0.8     |

### 3.3 Transfer learning from latency predictors to improve accuracy predictors

We demonstrate that latency predictors are surprisingly helpful in improving the training of an accuracy predictor – both in terms of absolute accuracy and the resulting NAS performance. The idea is that these GCN-based predictors for latency, accuracy and FLOPS have the same input representation. A trained GCN (e.g. for latency prediction) captures features of a model which are also useful for a similar GCN trained to predict a different metric (e.g. accuracy).

To show that, we initialize the weights of an accuracy predictor with those from a latency/FLOPS predictor (Section 3.2). We then train the predictor using the validation accuracy of the CIFAR-100 dataset. All predictors are trained for 100 times, each time using a randomly sampled set of 100
models from the NAS-Bench-201 dataset. Another, 100 random models are used for validation and
the remaining 14k models are left for testing. As shown in Table 2, the quality of accuracy prediction
improves in all cases. In particular, the accuracy predictors with transfer learning from FLOPS, which
is freely available, can increase the sample efficiency by around 2 times. We note that the proposed
transfer learning method is applicable to any accuracy predictors with existing training techniques.
We refer to S.M. for the NAS results and analysis.

| Error bound | 50 samples | 100 samples | 200 samples |
|-------------|------------|-------------|-------------|
| Standard    | Init-GPU   | Init-FLOPS  | Standard    | Init-GPU   | Init-FLOPS  | Standard    |
| ±1%         | 22.1±3.3   | 26.3±3.8    | 25.3±4.1    | 27.5±3.9   | 32.0±4.1    | 32.3±3.8    | 34.6±2.9    |
| ±5%         | 72.7±3.0   | 74.8±3.4    | 73.7±3.6    | 76.9±2.4   | 80.5±2.2    | 80.5±2.7    | 81.7±1.8    |
| ±10%        | 85.4±2.4   | 87.0±2.7    | 87.2±2.4    | 88.2±1.7   | 90.4±1.6    | 91.0±2.0    | 90.8±1.3    |

4 Binary Relation Prediction-based NAS (BRP-NAS)

In the previous section, we assumed that the accuracy of the model is freely available during the
search and focused on the latency prediction. In practice, accuracy of the model is computationally
expensive to obtain, sometimes more than latency, as it requires training. The cost of NAS critically
depends on the sample efficiency, which reflects how many models need to be trained and evaluated
during the search.

In this section, we (a) propose a new prediction-based NAS framework, called Binary Relation
Predictor-based NAS (BRP-NAS in short), that combines a GCN binary relation predictor and a
novel iterative data selection strategy; (b) demonstrate that it vastly improves the sample efficiency
of NAS for accuracy optimization; and (c) show that, by combining BRP-NAS with our GCN latency
predictor, we can also improve the sample efficiency of NAS for latency constrained deployments.

4.1 Binary relation predictor-based NAS

We propose a new predictor-based NAS according to the following observations: (a) accuracy
prediction is not necessarily required to produce faithful estimates (in the absolute sense) as long
as the predicted accuracy preserves the ranking of the models; (b) any antisymmetric, transitive and
connex binary relation produces a linear ordering of its domain, implying that NAS could be solved
by learning binary relations, where \( O(n^2) \) training samples can be used from \( n \) measurements; (c)
accurately predicting the rankings of top candidates is the most important. (We refer to the S.M. for a
more formal discussion on these observations and intuition behind them.)

BRP-NAS consists of two phases. In the first phase, the ranking of all candidate models is predicted
based on the outputs from a binary relation predictor, which is trained to predict the binary relation
(accuracy comparisons between two models). In the second phase, based on the predicted rankings,
models with high predicted ranks are fully trained, after which, the model with the highest trained
accuracy is selected.

**Binary relation predictor.** We propose a GCN based approach to learn a binary relation for NAS,
as illustrated in Figure 5. The predictor reuses the GCN part of the latency predictor, without any
changes, to generate graph embeddings for both input models. The embeddings are then concatenated
and passed as input to a fully connected layer which produces a 2-valued vector. The vector is then
passed through a softmax function to construct a simple probability distribution \( p = (p_1, p_2) \in \mathbb{R}^2 \)
with \( p_1 \) being the probability of the first model being better than the second, and \( p_2 \) being the
probability of the opposite. The produced probability distribution is then compared to the target
probability distribution obtained by taking a softmax of the ground-truth accuracy of the two models
\( (T_1, T_2) \), and the objective is to minimize the KL divergence between the two distributions. The
overall network structure and the loss function are summarized in Figure 5.
Training via iterative data selection. Given a budget of $T$ models which can be trained and $I$ iterations, we start by randomly sampling and training $T/I$ models from the search space which will be used to train the initial version of the predictor. At the beginning of each following iteration, we use the predictor to estimate the accuracy of all the models, denoted by $M$, in the search space. We then select the top $\alpha \ast T/I$ unique models and randomly pick another $(1 - \alpha) \ast T/I$ models from the top $M/2^i$ models where $\alpha$ is a factor between 0 and 1 and $i$ is the iteration counter. The selected $T/I$ models are trained and their resulting accuracies are used to further train the predictor for the next iteration. Tuning $\alpha$ results in a trade-off between exploitation and exploration and we use $\alpha = 0.5$ for all our experiments. We demonstrate that this iterative data selection plays an important role in achieving a significant performance gain (Figure 5).

Results. Figure 5 shows the advantages of the proposed binary relation and iterative data selection in BRP-NAS. Specifically, although the correlation between the measured ranking and the ground truth ranking decreases with iterative data selection (middle vs right), BRP-NAS is able to find better models because it focuses on high performing models only. Figure 5 on the other hand, shows that BRP-NAS outperforms previous methods, such as aging evolution [24], REINFORCE [5], and random sampling, by being up to $3x$ more sample efficient. The dotted vertical black line represents the point at which the prediction was trained up to. Due to the greediness of BRP-NAS, it is able to aggressively search for better models after the first iteration, increasing its exploitation and reducing its exploration every following iterations.

Comparison to Prior Work on NAS-Bench-101. To gauge the efficiency and quality of our BRP-NAS, we compare to previously published work. Simultaneously, this comparison shows how our technique scales to much larger benchmarks as we use NAS-Bench-101 [28] with over 423k points. Table 3 shows the result of this comparison, both in terms of the total number of trained models (a measure of algorithm speed) and final test accuracy (indicating algorithm quality). We train BRP-NAS using the validation accuracy from 100 models then we train the top 45 models returned
by the predictor. With a total of 145 trained models we are able to find a more accurate model faster than any previous work, as highlighted in Table 3.

| # Training Points | NAO [18] | Wen et al. [11] | NPENAS [10] | BRP-NAS (ours) |
|-------------------|-----------|----------------|-------------|---------------|
| Final Test Accuracy [%] | 1000      | 256           | 150         | 145           |
|                    | 93.73     | 94.12         | 94.14       | 94.16         |

### 4.2 BRP-NAS for latency constrained deployments

We combine BRP-NAS together with our GCN-based latency predictor from Section 3 to further improve NAS performance in the latency constrained settings (as in Figure 2 in Section 3). We compare our BRP-NAS against Aging Evolution paired with layer-wise predictors, which combines the state-of-the-art (SOTA) latency predictor together with the SOTA NAS algorithm. Our results demonstrate that the naive combination is far from optimal.

![Figure 6: BRP-NAS outperforms Aging Evolution (current state-of-the-art) and other popular search methodologies on NAS-Bench-201 without latency constraints (left) and with 5ms latency constraints (right). For the constrained case, desktop GPU was used and the SOTA Aging Evolution was paired with a baseline layer-wise model.](image)

### 5 Latency Benchmark

In this section, we present LatBench – a latency dataset of NAS-Bench-201 models on a wide range of devices. Similar to the motivations of NAS-Bench-101 and NAS-Bench-201, we aim towards (a) reproducibility and comparability in hardware-aware NAS and (b) ameliorating the need for researchers to have access to a broad range of devices. Although Nas-Bench-201 provides computational metrics such as number of parameters, FLOPS, and latency, these metrics are computed with operations and skip connections that do not contribute to the resulting output, leading to inaccurate measurements. Additionally, as latencies among devices often have weak correlations, more devices are required to facilitate the research of hardware-aware NAS.

We first remove any dangling nodes and edges and run each model in NAS-Bench-201 on the follow devices: (i) Desktop CPU - Intel(R) Core(TM) i7-7820X, (ii) Desktop GPU - NVIDIA GTX 1080 Ti, (iii) Embedded GPU - NVIDIA Jetson Nano, (iv) Embedded TPU - Google EdgeTPU, (v) Mobile GPU - Qualcomm Adreno 612 GPU, (vi) Mobile DSP - Qualcomm Snapdragon 855 DSP.

Specifically, we run each model 1000 times on each aforementioned non-mobile device using a patch size of $32 \times 32$ and a batch size of 1. For mobile devices, each model is run 10 time with the same settings. In order to lessen the impact of any startup/cool-down effects such as the creation and loading of inputs into buffer, we discard latencies that fall outside the lower and higher quartile values before taking the average of every 10 runs. These averages are discarded again with the aforementioned thresholds before a final average is taken.

For more details and further analysis of LatBench, please refer to our S.M. We also provide the FLOPS and the number of parameters for these models after removing unneeded nodes and edges. We have plans of updating LatBench by adding more devices in the future.
6 Conclusion

We introduced BRP-NAS, a new prediction-based NAS framework that combines a binary relative accuracy predictor architecture and an iterative data selection strategy to improve the performance of NAS. BRP-NAS outperforms previous NAS methods in both sample efficiency and accuracy for NAS-Bench-101 and NAS-Bench-201 benchmarks. We also release LatBench – a latency dataset for models in the NAS-Bench-201 on different devices.

Broader Impact

This research can democratize on-device deployment with cost-efficient NAS methodology for model optimization within device latency constraints. Additionally, carbon footprint of traditionally expensive NAS methods is vastly reduced. On the other hand, measurement and benchmarking data can be used both to create new NAS methodologies, and to gain further insights about the device performance. This can bridge the machine learning and device research communities together.

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Supplementary Material

S1 Supplementary Material for Section 3: Latency Prediction in NAS

S1.1 Neural network models supported by GCN predictor

GCN can handle any set of neural network models. In this paper, we apply GCN to NAS-Bench-201 and NAS-Bench-101. Their network structures are described below.

In NAS-Bench-201, the skeleton of any model consists of 3 stacks of 5 cells with a fixed structure and placeholders for 6 operation nodes. In the original paper, this cell structure is described with the help of a directed acyclic graph whose nodes and edges represent tensors and data dependencies between them, respectively. Additionally, each edge is also assigned a label which defines the operation to apply to the source tensor and whose result is used to define the content of the destination tensor. Since the structure of the cell is fixed, the only "searchable" part of the cell are labels to be assigned to the edges – the authors considered 5 different options for each label: 'zero' operation, "identity" operation (a.k.a. skip-connection), convolution $3 \times 3$, convolution $1 \times 1$, and $3 \times 3$ average pooling. Therefore, each architecture in NAS-Bench-201 can be defined by selecting 6 elements (with repetitions) from the aforementioned set of operations ($O_i$ for $i = 1...6$) and represented with an architecture string: $|O_1\sim0|+|O_2\sim0|O_3\sim1|+|O_4\sim0|O_5\sim1|O_6\sim2|$ (as defined by the NAS-Bench-201 authors).

For the purpose of this work, we have modified the representation of the models in NAS-Bench-201 dataset in the following way:

- When constructing the graph representation of a network to use it with our GCN predictors, we begin by converting the NAS-Bench-201 cell graph (Figure S1 left) into its equivalent form using more traditional convention where nodes represent operations (Figure S1 middle);
- We optimize the graph by completely detaching "zero" and "skip-connect" operations, and then removing all other nodes which became dangling (i.e., they do not lay on the path from input to output) because of the previous step;
- As mentioned in Section S2, we add a global node which is connected to all other nodes (including the nodes which were detached due to optimizations) and also add self-connections for all nodes – this results in an adjacency matrix (Figure S1 right) with dimensions $9 \times 9$ (6 operation nodes, "input", "output" and "global" node) which is one of the inputs to the GCN;
- Finally, for each node we construct its feature vector by encoding the node’s type using a one-hot vector – because "zero" and "skip-connect" operations were optimized out the possible choices are: the three remaining operations plus "input", "output" and "global" node types – thus the feature matrix is $9 \times 6$.

In NAS-Bench-101, modules are represented by directed acyclic graphs with up to 7 nodes. The valid operations at each node are convolution $3 \times 3$, convolution $1 \times 1$, and $3 \times 3$ max pooling. This results in an adjacency matrix with dimensions $8 \times 8$ (5 operation nodes, "input", "output" and "global" node) and a feature matrix with dimensions $8 \times 6$ (3 operations plus "input", "output" and "global" node types).

S1.2 Latency predictor for various devices

Table S2 and Figure S1 show the performance of the proposed GCN predictor. We first train each predictor for 100 times, each time using the hyperparameters summarized in Table S1 and a randomly sampled set of 900 models in the NAS-Bench-201 dataset. 100 models are used for validation and the remaining 14k models are used for testing. Values reported in Table S2 are the percentage of models in the test set that the predicted latency is within the corresponding error bound of the measured latency. The GCN predictors generalize well to unseen models in the NAS-Bench-201 dataset, and significantly outperform layer-wise predictors. We also see that the strong performance generalizes across various devices, which have vastly different latency behaviors. Then we experiment with training the GCN predictors using a randomly sampled set of 100 models. The performance degrades but still outperform the layer-wise predictors.

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1 One of the reasons behind this decision was to have a unified network representation consistent between NAS-Bench-101 and 201.

2 For skip-connections, before detaching we make sure that all direct predecessors of the node are instead connected directly to all direct successors of the node.

3 Since the optimized nodes are actually still present in the graph (but detached from anything else) we simply considered them "typeless" and assign zeros-only vectors to them.
Figure S1: (Left) Graph representation of a cell used in NAS-Bench-201 models, as defined by the authors, (Middle, Right) equivalent representation (with additional global node) and its adjacency matrix (without considering optimizations to remove "zero" and "skip-connect" operations) which are used in this paper.

Table S1: Training hyperparameters of the latency predictors.

| Hyperparameter         | Value                        | Notes                                      |
|------------------------|------------------------------|--------------------------------------------|
| Batch size             | 10                           |                                             |
| Learning rate schedule | plateau (reduce learning rate by half if no improvement is seen for 10 epochs) |                                             |
| Initial learning rate  | 0.0008                       |                                             |
| Optimizer              | AdamW                        |                                             |
| L2 weight decay        | 0.0005                       |                                             |
| Dropout ratio          | 0.002                        |                                             |
| Training epochs        | 250 (early stopping patience of 35 epochs) |                                             |

Table S2: Performance of latency predictors of various devices on NAS-Bench-201: (i) D. CPU - Intel(R) Core(TM) i7-7820X, (ii) D. GPU - NVIDIA GTX 1080 Ti, (iii) E. GPU - NVIDIA Jetson Nano, (iv) E. TPU - Google EdgeTPU, (v) M. GPU - Qualcomm Adreno 612 GPU, (vi) M. DSP - Qualcomm Snapdragon 855 DSP.

| Error bounds | Accuracy [%] | D. CPU | D. GPU | E. GPU | E. TPU | M. GPU | M. DSP |
|--------------|--------------|--------|--------|--------|--------|--------|--------|
| **GCN (900 pts.)** |              |        |        |        |        |        |        |
| ±1%          | 36.0±3.5     | 36.7±4.0 | 24.3±1.4 | 16.2±3.6 | 17.5±2.8 | 21.3±1.9 |
| ±5%          | 85.2±1.8     | 85.9±1.9 | 82.5±1.5 | 64.0±5.7 | 67.5±7.4 | 77.5±2.6 |
| ±10%         | 96.4±0.7     | 96.4±0.7 | 96.3±0.5 | 87.4±2.7 | 90.5±5.5 | 94.2±0.4 |
| **GCN (100 pts.)** |              |        |        |        |        |        |        |
| ±1%          | 6.1±1.7      | 5.9±1.3 | 9.9±1.3 | 6.2±1.0 | 5.2±0.9 | 10.3±1.1 |
| ±5%          | 27.9±5.5     | 28.7±3.6 | 44.6±4.0 | 30.0±3.6 | 24.9±3.4 | 48.0±3.8 |
| ±10%         | 51.5±8.3     | 52.9±5.0 | 71.8±3.5 | 54.6±5.7 | 46.3±4.1 | 78.4±3.6 |
| **Layer-wise (900 pts.)** |              |        |        |        |        |        |        |
| ±1%          | 3.5±0.2      | 4.2±0.2 | 6.1±0.3 | N/A    | N/A    | N/A    |
| ±5%          | 18.2±1.5     | 17.1±0.3 | 29.7±0.8 | N/A    | N/A    | N/A    |
| ±10%         | 29.6±1.1     | 32.6±1.2 | 54.0±0.8 | N/A    | N/A    | N/A    |

S1.3 Oracle NAS

In this section, we provide a detailed description of oracle NAS and the comparison between the layer-wise latency predictor-based oracle NAS and our GCN latency predictor-based oracle NAS (Figure S2). As noted in Section 3.1, in order to analyze the error introduced by an inaccurate latency estimation on NAS, we consider a
set of experiments where a perfect searching algorithm, denoted by oracle NAS, is used to find the best possible model under a varying latency threshold. Here “perfect” means that the algorithm has the full knowledge about accuracy of all points and is always able to find the most accurate one, but its knowledge about latency of different models is potentially limited by how latency is estimated. For each latency threshold \( l_{th} \) we begin by discarding all models which are believed to be too expensive according to the latency predictor in use. We then obtain the best model out of those which are left using our oracle search – this model is the assumed best but we are still not sure because it might have been falsely accepted due to imperfect latency estimation. Therefore we re-validate the assumed best model, this time using its measured latency, and only accept it if it truly falls below the latency limit. Otherwise we call it a false positive and discard it, repeating the aforementioned process with the second best point according to the initial search result. The first model encountered during this re-validation phase whose latency falls below the threshold is called the effective best for a given predictor with latency limit, and the effective best of a search when the ground-truth measured latency is always used is called ground-truth best.

As shown in Figure S2, we extensively study the difference between the assumed best and the effective best (introduced by false positives), as well as the difference between the accuracy of the ground-truth best and the effective best (introduced by false negatives) and some other accompanying metrics. Formally, for a set of models \( S \), a latency threshold \( l_{th} \), latency predictor \( \text{pred}() \) and measured latency \( \text{lat}() \), we can define: (i) the set of false positives: \( \{ s \mid s \in S \land \text{pred}(s) < l_{th} \land \text{lat}(s) > l_{th} \} \); (ii) the set of false negatives: \( \text{pred}(s) > l_{th} \land \text{lat}(s) < l_{th} \); (iii) analogically true positives/negatives if comparison with \( l_{th} \) is consistent between \( \text{pred}() \) and \( \text{lat}() \); (iv) and finally the set of truly positive points when \( \text{lat}(s) < l_{th} \).

Let us denote the set of: false/true negatives as \( N_f \) and \( N_t \) respectively, analogically false and true positives as \( P_f \) and \( P_t \), and the set of truly positives as \( P \). The assumed best is defined as: \( s^*_f = \arg \max_{s \in P_f \cup P_t} \text{accuracy}(s) \); effective best as: \( s^*_p = \arg \max_{s \in P_t} \text{accuracy}(s) \); and ground-truth best as: \( s^* = \arg \max_{s \in P} \text{accuracy}(s) \). Then, Figure S2 shows the following metrics as functions of latency threshold:

- Top left: the number of false positives denotes how many models were considered below the limit incorrectly, i.e. \( |P_f| \).
- Top right: the number of false negatives denotes how many models were considered above the limit incorrectly, i.e. \( |N_f| \).
- Middle left: the missed accuracy denotes the accuracy difference between the ground-truth best model and the effective best model, i.e. \( \text{accuracy}(s^*) - \text{accuracy}(s^*_p) \).
- Middle right: the related latency prediction error if a model was missed, i.e. \[
\begin{cases}
\text{pred}(s^*) - \text{lat}(s^*) & \text{if } s^* \neq s^*_p \\
0 & \text{otherwise}
\end{cases}
\]
Figure S2: Oracle NAS results for desktop GPU, using GCN and Layer-wise latency predictors. Results are obtained on the NAS-Bench-201 dataset for desktop-GPU using both the layer-wise and GCN-based latency predictors. All latency thresholds are between 1-7ms with a step size of 0.1ms.

- Bottom left: the over-claimed accuracy denotes the accuracy difference between the assumed best model (i.e. including false positives) and the effective best model after removing false positives, i.e. \( \text{accuracy}(s_p^*) - \text{accuracy}(s_f^*) \)
- Bottom right: the related latency prediction error if a model was over-claimed, i.e.
  \[
  \begin{cases} 
  \text{pred}(s_f^*) - \text{lat}(s_f^*) & \text{if } s_f^* \neq s_p^* \\
  0 & \text{otherwise}
  \end{cases}
  \]

S1.4 Transfer learning from latency predictors to improve accuracy predictors

Latency predictors can improve the performance of accuracy predictor as shown in Table 2 of Section 3. The trained GCN captures the correlated features in the model which is useful to guide the training of a different GCN. Figure S3 further shows that the training process is improved. Y-axis is the percentage of models with predicted validation accuracy within the error bound relative to the actual validation accuracy. When initialized with the weight of latency/FLOPS predictor, the training process of accuracy predictor converges faster to better results.

In order to understand the underlying behavior and to improve the accuracy predictor proposed in Section 3.3, we plot the rankings produced by a standard predictor-based search (Figure S4 left) and by a predictor transferred from latency predictor against the ground-truth ranking (Figure S4 right). Even though the accuracy predictor with transferred knowledge performs better in predicting the accuracy values of the models overall, the gain in accuracy ranking (which is important to NAS performance) is not as much. This motivates BRP-NAS described in Section 4.
Figure S3: Training curves of the accuracy predictors without transfer learning (standard), with transfer learning from desktop GPU latency predictor (Init-GPU), and with transfer learning from FLOPS predictor (Init-FLOPS).

Figure S4: (Left) Rankings produced by a standard predictor-based search. (Right) ranking produced by a predictor transferred from a latency predictor, x-axis is the position of a model according to the ground-truth ranking using validation accuracy, y-axis represents the average position of model in a ranking produced by a relevant method and the dashed red line marks the $x = y$ diagonal (i.e., perfect ranking).

S2 Supplementary Material for Section 4: BRP-NAS

S2.1 Motivation behind binary relation predictors.

We propose the binary relation predictor in Section 4 based on the following observations and intuition.

Observation 1: Ranking candidate models correctly according to their accuracy is more important than improving the absolute average accuracy of the accuracy predictor.

When the number of training samples is to be minimized, like in NAS – the prediction quality of a GCN accuracy predictor can be improved by considering cheaper but roughly-correlated metrics, such as latency or FLOPS. However, even when using those cheaper metrics, the achievable prediction accuracy degrades significantly as the number of training samples becomes heavily limited as shown in Table 2 of Section 3. In order to maintain decent NAS quality even in those extreme cases, we propose to make more fundamental (compared to naively increasing a predictor’s accuracy) changes in the predictor-based NAS by relaxing some of the current assumptions behind it.

More formally, we consider a predictor which gives each model a score rather than predicts the absolute accuracy a model. Let $P$ be the predicted order of models obtained from the estimated scores, i.e. $P_n$ is the model in the search space which achieves the $n$-th largest score as estimated by a predictor. Consequently, let $GT$ be the ground-truth order, i.e. $GT_n$ is the model which achieves the $n$-th highest validation accuracy. Furthermore, let $P(GT_n)$ be the position in $P$ of the $GT_n$ model, i.e. $P(GT_n) = m \iff P_m = GT_n$. Similarly, $GT(P_n)$ is the analogical reverse. It is easy to see that the performance of our predictor-based NAS should be maximized when $P = GT$, regardless of the values predicted by the scoring function. Although a perfect accuracy predictor (in the absolute sense) would produce the perfect ordering of models, we argue that learning the perfect accuracy function is more challenging than learning a function which is only supposed to produce faithful ordering of models.
Observation 2: Learning a binary relation rather than predicting absolute models.

Taking a step further, the predicted order $P$ even need not be produced by a scoring function. Instead, we lean on the fact that any antisymmetric, transitive and connex binary relation produces a linear ordering of its domain. Thus, NAS could be solved by learning a binary relation rather than predicting absolute models. This is a very important observation to maximize sample efficiency, since the reformulated binary relation changes the number of training samples for the predictor in a function of trained models to $O(n^2)$, rather than $O(n)$ in the standard approach. This provides the predictor with more opportunities to learn efficiently when $n$ is limited.

We quantify the quality of different rankings $P$ produced by the proposed binary relation predictor together with different variations of the standard predictor. All predictors are trained for 200 times, each time using a randomly sampled set of 100 models. Then they are used to sort all 15k models in the NAS-Bench-201 dataset to produce a ranking. We have compared the predicted rankings by considering their correlation to the GT rankings in Figure 5 (middle) of Section 4. The average Spearman-ρ correlation coefficient between the position in prediction ranking and that in GT ranking shows that the proposed binary relation predictor achieves the best ranking correlation out of all our experiments. However, despite producing the best results globally, the binary predictor does not yield the best NAS results. This leads to the next observation.

Observation 3. Top-K rankings are important.

Even though $P = GT$ maximizes the performance of predictor-based NAS, achieving perfect correlation between the two rankings is very challenging in practice considering a limited number of training samples. Although errors are expected to occur somewhere in the predicted ranking, in the context of NAS, we can make sure that those errors are minimized in the top of the rankings, otherwise even a very well correlated ranking might fall short to a less optimal alternative.

When closely examining the results obtained by running the binary relation predictor, we see that even though the global correlation is very good, the best performing models happen to be burdened with a relatively higher error than the rest of the search space, as indicated by the red circle in Figure 5. In the context of NAS, any ranking $P'$ which satisfies $P'_1 = GT_1$ is as good as the perfectly correlated ranking $P = GT$, and analogically, any ranking $P''$ for which $GT(P''_1)$ is very high is less likely to yield good results in practice, regardless of their global landscapes.

Section 4 has introduced BRP-NAS - a NAS method based on binary relation predictor combined with an iterative data selection strategy. Algorithm 1 describes the steps to search for the best model based on pairwise relation learning and to find better models by focusing on high performing models. Figure S5 shows that the proposed method achieves the best NAS performance. The iterative training approach helps with the top model performance even though achieves worse results globally.

S2.2 Details on NAS algorithms used in the paper

Predictor-based NAS. We train each predictor using the hyperparameters listed in Table S3.

For all NAS experiments, the training set for predictors was discovered online (i.e., no prior knowledge was assumed), therefore, we did not have access to a separate validation set – whenever a validation set would have been used, we used training set instead.

To perform NAS with our predictor, in the first phase, we use a randomly selected small set of $K$ models from the search space to train the predictor (with or without iterative data selection). Then in the second phase, we use the predictor to score all the models in the search space in order to find potentially the most efficient one. The predictor could be trained in the second phase if required, but we did not do that in order to check the achievable performance when $K$ is upper-bounded.

When training the predictor iteratively, we always use 5 iterations. It means that different number of models ($K/5$) were trained and added to the predictor’s training set in each iteration.

Figure S5 summarizes the results of NAS using various predictors. BRP-NAS, which utilizes binary relation predictor trained via iterative data selection, has the best performance comparing to other approaches.

Aging Evolution. We run aging evolution with pool size 64 and sample size 16, values which we found work well for NAS-Bench-201 models.

REINFORCE. Similar to [1], we use a single cell LSTM controller which is trained with REINFORCE (no PPO).

Random search. We pick models randomly by picking 6 numbers from the range of 1-5 uniformly.
Algorithm 1: The proposed search method based on pairwise relation learning.

**Input:** (i) Search space $S$, (ii) budget for predictor training $K$ (number of models), (iii) number of iterations $I$, (iv) latency limit $L_{\text{max}}$ and latency predictor $P_L$, (v) trade-off factor $\alpha$ between 0 and 1, (vi) number of models to test after predictor is trained $M$.

**Output:** The best found model $s^*$

1. $C \leftarrow \{ s \mid s \in S \land \text{predicted\_latency}(s) \leq L_{\text{max}} \}$
2. $T \leftarrow \emptyset$
3. $BP \leftarrow$ initialize binary predictor with weights from $P_L$
4. **for** $i \leftarrow 1$ **to** $I$ **do**
5. $M \leftarrow \{ \text{select the top } \alpha \cdot K/I \text{ models and randomly select } (1 - \alpha) \cdot K/I \text{ models from } C \text{ which are not already in } T \}$
6. **foreach** $m \in M$ **do**
7. $a \leftarrow \text{train\_and\_validate}(m)$
8. $T \leftarrow T \cup (m, a)$
9. **end**
10. **foreach** $(m_1, a_1), (m_2, a_2) \in T \text{ s.t. } m_1 \neq m_2$ **do**
11. $l \leftarrow \text{softmax}(BP(m_1, m_2))$
12. $t \leftarrow \text{softmax}([a_1, a_2])$
13. optimize $BP$ to minimize KL-divergence between $t$ and $l$
14. **end**
15. $C \leftarrow \text{sort } C \text{ using } BP \text{ to compare models and take the upper half (discard the rest)}$
16. **end**
17. $S \leftarrow \text{sort } S \text{ using } BP$
18. $s^* \leftarrow \text{NONE}$
19. **foreach** $m \in S$ **do**
20. **if** $\text{latency}(m) \leq L_{\text{max}}$ **then**
21. train and evaluate $m$, update $s^*$ if $m$ happens to be better than the best model so far
22. **end**
23. **end**

Table S3: Training hyperparameters of the accuracy predictors.

| batch size | K=100 | K=50 | K=25 |
|-----------|-------|------|------|
| normal    | 50    | 32   | 16   |
| binary    | 64    | 32   | 32   |

Learning rate schedule: cosine annealing

Initial learning rate: 0.00035

Optimizer: AdamW

L2 weight decay: 0.0005

Dropout ratio: 0.2

Training epochs: 250 (early stopping patience of 35 epochs)

Figure S5: (Left) Comparison of NAS performance with the standard GCN predictor, GCN predictor with transfer learning (from desktop GPU, Embedded TPU and FLOPS predictors) and BRP-NAS, all trained non-iteratively. (Middle, Right) Comparison with predictors trained via iterative approach with $\alpha = 0$ (middle) and $\alpha = 0.5$ (right).
S2.3 Comparison to Prior Work on NAS-Bench-101.

We compare BRP-NAS with the previously published prediction-based NAS on NAS-Bench-101. We first train the predictor using the validation accuracy from 100 models, then we train the subsequent models which are picked from the top-ranked models returned by the predictor. As shown in Figure S6, BRP-NAS finds a model with higher final test accuracy (94.16%) using fewer steps (145 trained models) than the work under comparison.

Figure S6: Comparison to prior work on NAS-Bench-101 dataset.

S3 Supplementary Material for Section 5: Latency Benchmark

In Figure S6, we show the scatter plots of models taken from NAS-Bench-201 dataset that illustrates the connection between the latency of various devices and FLOPS/number of parameters. Each point in the plots represents the average latency of running a model on the stated device. We can see that latency is not strongly correlated with FLOPS or number of parameters. These metrics are unreliable proxies to predict latency.

Figure S6 and Table S4 illustrate the latency correlation between devices. Most of the metrics are not strongly correlated which indicates that having a dedicated latency predictor trained for each class of devices is necessary to provide good latency estimation. This motivates us to provide LatBench as a latency dataset.

Figure S6: In most cases, FLOPS and the number of parameters are not a good approximation towards run-time latency on-device.
Figure S6: Latency differs for each class of devices.
Table S4: Latency correlation between various devices.

|       | D. CPU | D. GPU | E. GPU | E. TPU | M. GPU | M. DSP |
|-------|--------|--------|--------|--------|--------|--------|
| D. CPU| 1.000  | 0.997  | 0.700  | 0.844  | 0.751  | 0.727  |
| D. GPU| 0.997  | 1.000  | 0.702  | 0.844  | 0.752  | 0.728  |
| E. GPU| 0.700  | 0.702  | 1.000  | 0.574  | 0.866  | 0.821  |
| E. TPU| 0.844  | 0.844  | 0.574  | 1.000  | 0.548  | 0.690  |
| M. GPU| 0.751  | 0.752  | 0.866  | 0.548  | 1.000  | 0.821  |
| M. DSP| 0.727  | 0.728  | 0.821  | 0.690  | 0.821  | 1.000  |