TOWARDS DISCOVERING NEURAL ARCHITECTURES FROM SCRATCH

Anonymous authors
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ABSTRACT

The discovery of neural architectures from scratch is the long-standing goal of Neural Architecture Search (NAS). Searching over a wide spectrum of neural architectures can facilitate the discovery of previously unconsidered but well-performing architectures. In this work, we take a large step towards discovering neural architectures from scratch by expressing architectures algebraically. This algebraic view leads to a more general method for designing search spaces, which allows us to compactly represent search spaces that are 100s of orders of magnitude larger than common spaces from the literature. Further, we propose a Bayesian Optimization strategy to efficiently search over such huge spaces, and demonstrate empirically that both our search space design and our search strategy can be superior to existing baselines. We open source our algebraic NAS approach and provide APIs for PyTorch and TensorFlow.

1 INTRODUCTION

Neural Architecture Search (NAS), a field with over $1\,000$ papers in the last two years (Deng & Lindauer, 2022), is widely touted to automatically discover novel, well-performing architectural patterns. However, while state-of-the-art performance has already been demonstrated in hundreds of NAS papers (prominently, e.g., (Tan & Le, 2019; 2021; Liu et al., 2019a)), success in automatically finding truly novel architectural patterns has been very scarce (Ramachandran et al., 2017; Liu et al., 2020). For example, novel architectures, such as transformers (Vaswani et al., 2017; Dosovitskiy et al., 2021) have been crafted manually and were *not* found by NAS.

There is an accumulating amount of evidence that over-engineered, restrictive search spaces (e.g., cell-based ones) are major impediments for NAS to discover truly novel architectures. Yang et al. (2020b) showed that in the DARTS search space (Liu et al., 2019b) the manually-defined macro architecture is more important than the searched cells, while Xie et al. (2019) and Ru et al. (2020) achieved competitive performance with randomly wired neural architectures that do not adhere to common search space limitations. As a result, there are increasing efforts to break these impediments, and the discovery of novel neural architectures has been referred to as the holy grail of NAS.

Hierarchical search spaces are a promising step towards this holy grail. In an initial work, Liu et al. (2018) proposed a hierarchical cell, which is shared across a fixed macro architecture, imitating the compositional neural architecture design pattern widely used by human experts. However, subsequent works showed the importance of both layer diversity (Tan & Le, 2019) and macro architecture (Xie et al., 2019; Ru et al., 2020).

In this work, we introduce a general formalism for the representation of hierarchical search spaces, allowing both for layer diversity and a flexible macro architecture. The key observation is that any neural architecture can be represented algebraically; e.g., two residual blocks followed by a fully-connected layer in a linear macro topology can be represented as the algebraic term

$$\texttt{Linear(Residual(conv, id, conv), Residual(conv, id, conv), fc)} \quad . \tag{1}$$

We build upon this observation and employ Context-Free Grammars (CFGs) to construct large spaces of such *algebraic architecture terms*. Although a particular search space is of course limited in its overall expressiveness, with this approach, we could effectively construct any neural architecture, facilitating the discovery of truly novel ones.

Due to the hierarchical structure of algebraic terms, the number of candidate neural architectures scales exponentially with the number of hierarchical levels, leading to search spaces 100s of orders of magnitudes larger than commonly used ones. To search in these huge spaces, we propose an efficient search strategy, Bayesian Optimization for Algebraic Neural Architecture Terms (BANAT), which leverages hierarchical information, capturing the topological patterns across the hierarchical levels, in its tailored kernel design.

Our contributions are as follows:

- We present an algebraic notion of NAS that views neural architectures as algebraic terms (Section 2).
- We propose to design spaces of these algebraic architecture terms using CFGs (Section 3).
- We propose BANAT, a Bayesian Optimization (BO) strategy that uses a tailored kernel to efficiently and effectively search over our huge search spaces (Section 4).
- After surveying related work (Section 5), we empirically show that search spaces of algebraic architecture terms perform on par or better than common cell-based spaces on different datasets, show the superiority of BANAT over common baselines, and demonstrate the importance of incorporating hierarchical information in the modeling (Section 6).

We open source our algebraic NAS approach and provide APIs for PyTorch (Paszke et al., 2019) and TensorFlow (Abadi et al., 2015) at `https://anonymous.4open.science/r/iclr23_tdnafs`.

2 ALGEBRAIC NEURAL ARCHITECTURE SEARCH

In this section, we develop an algebraic view on Neural Architecture Search (NAS) that we build upon in later sections.

Neural architectures as algebraic terms An algebra $(A, \mathcal{F})$ consists of a nonempty set A and operators $f\colon A^n \to A \in \mathcal{F}$ of different arities $n \geq 0$ (Birkhoff, 1935). In our case, A corresponds to the set of all (sub)architectures and we distinguish between two types of operators: (i) nullary operators which represent primitive computations (e.g., $\texttt{conv}()$ or $\texttt{fc}()$) and (ii) k-ary operators with $k > 0$ which represent topological operators (e.g., $\texttt{Linear}(\cdot,\cdot,\cdot)$ or $\texttt{Residual}(\cdot,\cdot,\cdot)$). For sake of notational simplicity, we omit parenthesis for nullary operators (i.e., we write `conv`).

More specifically, we introduce *algebraic architecture terms* as a string representation for neural architectures and propose to use term algebras, which map algebraic expressions to a string such as $f(g(h,k),h)$, where f, g, h, and k correspond to operators of arity 2 (f, h) and arity 0 (h, k), respectively. E.g., we can represent a neural architecture as the algebraic architecture term ω:

$$\omega = \texttt{Linear}(\texttt{Residual}(\texttt{conv},\ \texttt{id},\ \texttt{conv}),\ \texttt{Residual}(\texttt{conv},\ \texttt{id},\ \texttt{conv}),\ \texttt{fc}) \quad . \tag{2}$$

Crucially, term algebras also allow for variables x_i that can be set to terms themselves, e.g., $f(x_1, x_1) = f(g(h,k), g(h,k))$ for $x_1 = g(h,k)$. Therefore, we can introduce intermediate variables x_i to share structural patterns across the architecture. For example, we could define x_1 to map to the residual block in the above example as follows:

$$\omega' = \texttt{Linear}(x_1,\ x_1,\ \texttt{fc}), \quad x_1 = \texttt{Residual}(\texttt{conv},\ \texttt{id},\ \texttt{conv}) \quad . \tag{3}$$

Algebraic NAS Next, we formulate our algebraic view on NAS, where we search over algebraic architecture terms $\omega \in \Omega$ representing their associated architectures $\Phi(\omega)$:

$$\arg\min_{\omega \in \Omega} f(\Phi(\omega)) \qquad , \tag{4}$$

where $f(\cdot)$ is an error measure that we seek to minimize, e.g., validation error. For example, we can construct the popular cell-based NAS-Bench-201 search space (Dong & Yang, 2020) as follows: The search space consists of a fixed macro architecture $\texttt{Macro}(\ldots)$ that stacks 15 instances of a cell $\texttt{Cell}(\ldots)$; each cell has 6 edges for each of which one can choose from 5 primitive computations (i.e., p_i for $i \in \{1,\ 2,\ 3,\ 4,\ 5\}$ corresponding to `zero`, `id`, `conv1x1`, `conv3x3`, or `avg_pool`,

respectively). Further, we introduce the intermediate variable x_1 that effectively shares the cell structure across the architecture. Thus, we can express an architecture, e.g., $\langle 1, 2, 1, 5, 4, 3 \rangle$, from the NAS-Bench-201 search space as:

$$\omega = \texttt{Macro}(\underbrace{x_1, x_1, ..., x_1}_{15\times}), \quad x_1 = \texttt{Cell}(\underbrace{\texttt{p}_\texttt{i}, \texttt{p}_\texttt{i}, \texttt{p}_\texttt{i}, \texttt{p}_\texttt{i}, \texttt{p}_\texttt{i}, \texttt{p}_\texttt{i}}_{i \in \{1,\ 2,\ 3,\ 4,\ 5\}}) \quad . \tag{5}$$

Algebraic NAS over such algebraic architecture terms then amounts to finding the best-performing primitive computation $\texttt{p}_\texttt{i}$ for each edge, as the macro architecture is fixed. In contrast to this simple cell-based algebraic space, the search spaces we consider can be much more expressive and, e.g., allow for layer diversity and a flexible macro architecture over several hierarchical levels.

Even though the ideas above are very powerful, two questions immediately come to mind: (1) How to construct architecture term spaces Ω?, and (2) How to optimize over these huge spaces? In the following sections we take first steps towards answering these questions.

3 Constructing neural architecture terms with context-free grammars

To construct algebraic architecture terms, we utilize *Context-Free Grammars (CFGs)* (Chomsky, 1956) as these naturally generate (hierarchical) algebraic terms. Formally, a CFG $\mathcal{G} = \langle N, \Sigma, P, S \rangle$ consists of a finite set of nonterminals N, a finite set of terminals Σ (with $N \cap \Sigma = \emptyset$), a finite set of production rules $P = \{A \rightarrow \beta | A \in N, \beta \in (N \cup \Sigma)^*\}$, where the asterisk $*$ denotes the Kleene star operation (Kleene et al., 1956), and a start symbol $S \in N$. To generate an algebraic architecture term, starting from the start symbol S, we recursively replace nonterminals inside the current algebraic architecture term with a right-hand side of a production rule consisting of nonterminals and terminals, until the resulting string does not contain any nonterminals. For example, consider the following CFG in extended Backus-Naur form (Backus, 1959) (see Appendix B for a detailed description):

$$\text{S} \ ::= \texttt{Linear(S, S, S)} \mid \texttt{Residual(S, S, S)} \mid \texttt{conv} \mid \texttt{id} \mid \texttt{fc} \tag{6}$$

From this CFG, we can derive the algebraic neural architecture term (with three hierarchical levels) from Equation 2 as follows:

$$\begin{aligned} \text{S} &\rightarrow \texttt{Linear(S, S, S)} && \boxed{\text{Level 1}} \\ &\rightarrow \texttt{Linear(Residual(S, S, S), Residual(S, S, S), fc)} && \boxed{\text{Level 2}} \\ &\rightarrow \texttt{Linear(Residual(conv, id, conv), Residual(conv, id, conv), fc)} && \boxed{\text{Level 3}} \end{aligned} \tag{7}$$

Figure 1 makes the above derivation and the connection to the corresponding architecture explicit. The set of all (potentially infinite) algebraic terms generated by a CFG $\mathcal{G}$ is the language $L(\mathcal{G})$, which naturally forms our search space Ω. Thus, the algebraic NAS problem from Equation 4 becomes:

$$\arg\min_{\omega \in L(\mathcal{G})} f(\Phi(\omega)) \quad . \tag{8}$$

We can construct very expressive search spaces (e.g., see Section 6.1) as well as unify popular search spaces from the literature with our search space design (Appendix E). However, there is of course no single search space that can construct any neural architecture. I.e., architectures in our search space are limited to context-free languages; e.g., architectures of the type $\{a^n b^n c^n | n \in \mathbb{N}_{>0}\}$ cannot be generated by CFGs (this can be shown using Odgen's lemma (Ogden, 1968)).

Below, we augment the capabilities of CFGs and leverage properties of context-free languages so that we can incorporate constraints, foster regularity, and handle changes in the spatial resolution (and number of channels).

Constraints In many search space settings, we want to adhere to some constraints, e.g., to limit the number of nodes or to ensure that for all architectures in the search space there exists at least one path from the input to the output. We can simply do so by allowing only the application of production rules which guarantee compliance to such constraints. For example, to ensure that there is at least one path from the input to the output, it is sufficient to ensure that each derivation connects its input to the output due to the recursive nature of CFGs. Note that this makes CFGs context-sensitive w.r.t. those constraints. For more details please refer to Appendix D.

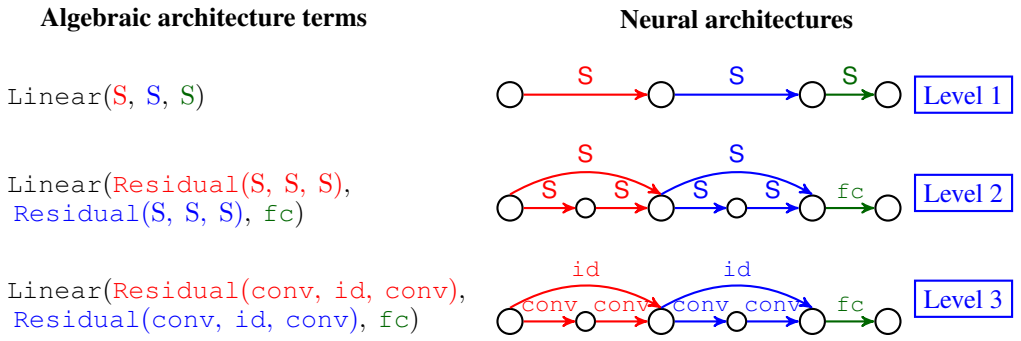

Figure 1: Derivations (see Equation 7) of algebraic terms (left) correspond to edge replacements (Habel & Kreowski, 1983; 1987; Drewes et al., 1997) in the associated neural architecture (right). Please refer to Appendix A for the vocabulary of topological operators and primitive computations.

Fostering regularity through substitution To implement intermediate variables x_i as described in Section 2, we utilize that context-free languages are closed under substitution: we map terminals, represented by the intermediate variables x_i, from one language to algebraic terms of other languages, e.g., a shared cell. For example, consider two CFGs $\mathcal{G}_1$ and $\mathcal{G}_2$. We can add intermediate terminals $x_1, x_2, ..., x_k$ to $\mathcal{G}_1$, each of which map to an algebraic term $\omega_1, \omega_2, ..., \omega_k \in L(\mathcal{G}_2)$. We can extend this notion by adding further intermediate terminals which map to other languages $L(\mathcal{G}_j)$, or by adding intermediate terminals to $\mathcal{G}_2$ which map to languages $L(\mathcal{G}_{j \neq 1})$. These algebraic terms are effectively shared across the architecture, fostering regularity.

For example, we can split a CFG $\mathcal{G}$, constructing entire algebraic architecture terms, into the CFGs $\mathcal{G}_{macro}$ and $\mathcal{G}_{cell}$ for the macro-level or cell-level, respectively. Further, we add a single terminal x_1 to $\mathcal{G}_{macro}$. In this way, we effectively search over the macro-level as well as a single, shared cell. Note that by using a fixed macro architecture, we can represent cell-based search spaces, e.g., NAS-Bench-201 (Dong & Yang, 2020), while also being able to represent more expressive search spaces (e.g., see Section 6.1).

Representing common architecture patterns for object recognition Neural architectures for object recognition commonly build a hierarchy of features that are gradually downsampled, e.g., by pooling operations. However, previous works in NAS were either limited to a fixed macro architecture (Zoph et al., 2018) or only allowed for linear macro architectures (Liu et al., 2019a). While this produced impressive performance on popular benchmarks (Tan & Le, 2019; 2021; Liu et al., 2019a), it is an open research question whether a different type of macro architecture (e.g., one with multiple branches) could yield even better performance.

To accommodate flexible macro architectures, we propose to overload the nonterminals to allow for spatial resolution changes in architectures with multiple branches. In particular, the nonterminals indicate how often we apply downsampling operations in the subsequent derivations of the nonterminal. Consider the production rule $\mathrm{D2} \rightarrow \texttt{Residual}(\mathrm{D1},\ \mathrm{D2},\ \mathrm{D1})$, where $\mathrm{D}i$ with $i \in \{1, 2\}$ are a nonterminals which indicate that i downsampling operations have to be applied in their subsequent derivations. That is, in both paths of the residual the input features will be downsampled twice and, consequently, the merging paths will have the same spatial resolution. Thus, this CFG design mechanism recursively distributes the downsampling operations over the architecture. For the channels, we adopted the common design to double the number of channels whenever we halve the spatial resolution. Note that we could easily handle a varying number of channels by using, e.g., depthwise concatenation as merge operation.

4 Bayesian Optimization for Algebraic Neural Architecture Search

We propose a BO strategy, Bayesian Optimization for Algebraic Neural Architecture Terms (BANAT), to search efficiently in the huge search spaces spanned by our algebraic architecture terms.

Bayesian Optimization BO is a family of efficient search techniques for finding the global optimum of a black-box objective problem, particularly when the objective is expensive to evaluate (Brochu et al., 2010; Frazier, 2018). At each BO iteration, a probabilistic surrogate is trained on the observed data to model the unknown objective problem. Based on this, an acquisition function is computed to score the utility of all the candidate points (e.g., architectures) and optimized to recommend the next point to evaluate.

Overview Our BO strategy for algebraic NAS, BANAT, introduces a novel surrogate model, which combines a Gaussian Process (GP) with a tailored kernel that leverages the hierarchical structure of algebraic neural architecture terms (see below), and adopts expected improvement as the acquisition function (Mockus et al., 1978). Given the discrete nature of our architecture search spaces, we optimize the acquisition function with an evolutionary algorithm. Furthermore, to reduce wallclock time by leveraging parallel computing resources, we adapt the Kriging Believer (Ginsbourger et al., 2010) to select architectures at every search iteration so that we can train and evaluate them in parallel. Specifically, it assigns hallucinated values to architectures that are already selected but not yet evaluated at each iteration to avoid redundant evaluations. For a more detailed explanation of the BO mechanism, please refer to Appendix F.

Hierarchical Weisfeiler-Lehman kernel (hWL) Inspired by the state-of-the-art BO approach for NAS (Ru et al., 2021), we adopt the WL graph kernel (Shervashidze et al., 2011) in a GP surrogate, modeling the architectures $\Phi(\omega_i)$ instead of its algebraic neural architecture terms ω_i. However, modeling solely based on the final architecture ignores the useful hierarchical information inherent in our algebraic representation. Moreover, the large size of the final architectures at the highest hierarchical level also makes it difficult to use a single WL kernel to capture the more global topological patterns.

Since our hierarchical construction of neural architectures can be viewed as a series of gradually unfolding architectures, with the final architecture containing only primitive computations (see Figure 1), we propose a novel hierarchical kernel design which assigns a WL kernel to each hierarchy and combines them in a weighted sum. To this end, we introduce fold operators F_l, that removes algebraic terms beyond the l-th hierarchical level. For example, for the algebraic term ω from Equation 2, the fold operators F_1, F_2 and F_3 yield

$$F_3(\omega) = \omega = \texttt{Linear}(\texttt{Residual}(\texttt{conv}, \texttt{id}, \texttt{conv}), \texttt{Residual}(\texttt{conv}, \texttt{id}, \texttt{conv}), \texttt{fc}), \tag{9}$$

$$F_2(\omega) = \texttt{Linear}(\texttt{Residual}, \texttt{Residual}, \texttt{fc}) \quad , \quad F_1(\omega) = \texttt{Linear} \quad .$$

Note the similarity to the derivations in Figure 1. Furthermore note that, in practice, we also add the corresponding nonterminals to integrate information from our construction process. Consider two architectures $\Phi(\omega_i)$ and $\Phi(\omega_j)$ with algebraic architecture terms ω_i and ω_j, respectively, constructed over a hierarchy of L levels. We then define our hierarchical kernel as follows:

$$k_{hWL}(\omega_i, \omega_j) = \sum_{l=2}^{L} \lambda_l \cdot k_{WL}(\Phi(F_l(\omega_i)), \Phi(F_l(\omega_j))) \qquad , \tag{10}$$

where the weights λ_l govern the importance of the learned graph information at different hierarchical levels and can be tuned (along with other hyperparameters of the GP) by maximizing the marginal likelihood. We omit $l = 1$ in the additive kernel as $F_1(\omega)$ does not contain any edge features which are required to apply our WL kernel k_{hWL}. Our proposed kernel can efficiently capture the information in all algebraic term construction levels, which substantially improves its empirical performance on our search space as demonstrated in Section 6.

Acquisition function optimization Top optimize the acquisition function in our BO strategy, we use an evolutionary algorithm. For the evolutionary operations, we adopt ideas from grammar-based genetic programming (McKay et al., 2010; Moss et al., 2020). For mutation operations, we randomly replace a sub-architecture term with a new randomly generated term, using the same nonterminal as start symbol. For crossover operations, we randomly swap two sub-architecture terms with the same corresponding nonterminal. We consider two crossover operators: a novel *self-crossover* operation swaps two sub-terms of a *single* architecture term, and the common crossover operation swaps sub-terms of two different architecture terms. Note that all evolutionary operations by design only result in valid terms. We provide examples for the evolutionary operations in Appendix F.

5 RELATED WORK

Neural Architecture Search Neural Architecture Search (NAS) aims to automatically discover architectural patterns (or even entire architectures) (Elsken et al., 2019). Previous approaches, e.g., used reinforcement learning (Zoph & Le, 2017; Pham et al., 2018), evolution (Real et al., 2017), gradient descent (Liu et al., 2019b), or Bayesian Optimization (BO) (Kandasamy et al., 2018; White et al., 2021; Ru et al., 2021). To enable the effective use of BO on graph-like inputs for NAS, previous works have proposed to use a GP with specialized kernels (Kandasamy et al., 2018; Ru et al., 2021), encoding schemes (Ying et al., 2019; White et al., 2021), or graph neural networks as surrogate model (Ma et al., 2019; Shi et al., 2020; Zhang et al., 2019). Different to prior works, we explicitly leverage the hierarchical construction of architectures for modeling.

Searching for novel architectural patterns Previous works mostly focused on finding a shared cell (Zoph et al., 2018) with a fixed macro architecture while only few works considered more expressive hierarchical search spaces (Liu et al., 2018; 2019a; Tan et al., 2019). The latter works considered hierarchical assembly (Liu et al., 2018), combination of a cell- and network-level search space (Liu et al., 2019a; Zhang et al., 2020), evolution of network topologies (Miikkulainen et al., 2019), factorization of the search space (Tan et al., 2019), parameterization of a hierarchy of random graph generators (Ru et al., 2020), a formal language over computational graphs (Negrinho et al., 2019), or a hierarchical construction of TensorFlow programs (So et al., 2021). Similarly, our formalism allows to design search spaces covering a general set of architecture design choices, but also permits the search for macro architectures with spatial resolution changes and multiple branches. We also handle spatial resolution changes without requiring post-hoc testing or resizing of the feature maps unlike prior works (Stanley & Miikkulainen, 2002; Miikkulainen et al., 2019; Stanley et al., 2019). Other works proposed approaches based on string rewriting systems (Kitano, 1990; Boers et al., 1993), cellular (or tree-structured) encoding schemes (Gruau, 1994; Luke & Spector, 1996; De Jong & Pollack, 2001; Cai et al., 2018), hyperedge replacement graph grammars Luerssen & Powers (2003); Luerssen (2005), attribute grammars (Mouret & Doncieux, 2008), CFGs (Jacob & Rehder, 1993; Couchet et al., 2007; Ahmadizar et al., 2015; Ahmad et al., 2019; Assunção et al., 2017; 2019; Lima et al., 2019; de la Fuente Castillo et al., 2020), or And-Or-grammars (Li et al., 2019). Different to these prior works, we construct entire architectures with spatial resolution changes across multiple branches, and propose techniques to incorporate constraints and foster regularity.

6 EXPERIMENTS

In this section, we investigate potential benefits of hierarchical search spaces and of our search strategy BANAT. More specifically, we address the following questions:

- **Q1** Can hierarchical search spaces yield on par or superior architectures compared to cell-based search spaces with a limited number of evaluations?
- **Q2** Can our search strategy BANAT improve performance over common baselines?
- **Q3** Does leveraging the hierarchical information improve performance?

To answer these questions, we introduce a hierarchical search space based on the popular NAS-Bench-201 search space (Dong & Yang, 2020) and experimentally answer them in the affirmative. We provide complementary results and analyses in Appendix G.

6.1 HIERARCHICAL NAS-BENCH-201

To answer the questions **Q1**-**Q3**, we introduce a hierarchical variant of the popular cell-based NAS-Bench-201 search space (Dong & Yang, 2020) by adding a hierarchical macro space (i.e., spatial resolution flow and wiring at the macro-level) and parameterizable convolutional blocks (i.e., choice of convolutions, activations, and normalizations). We express the hierarchical NAS-Bench-201 search

space with CFG $\mathcal{G}_h$ as follows:

$$
\begin{aligned}
\text{D2} &::= \texttt{Linear3(D1, D1, D0)} \mid \texttt{Linear3(D0, D1, D1)} \mid \texttt{Linear4(D1, D1, D0, D0)} \\
\text{D1} &::= \texttt{Linear3(C, C, D)} \mid \texttt{Linear4(C, C, C, D)} \mid \texttt{Residual3(C, C, D, D)} \\
\text{D0} &::= \texttt{Linear3(C, C, CL)} \mid \texttt{Linear4(C, C, C, CL)} \mid \texttt{Residual3(C, C, CL, CL)} \\
\text{D} &::= \texttt{Linear2(CL, down)} \mid \texttt{Linear3(CL, CL, down)} \mid \texttt{Residual2(C, down, down)} \\
\text{C} &::= \texttt{Linear2(CL, CL)} \mid \texttt{Linear3(CL, CL)} \mid \texttt{Residual2(CL, CL, CL)} \\
\text{CL} &::= \texttt{Cell(OP, OP, OP, OP, OP, OP)} \\
\text{OP} &::= \texttt{zero} \mid \texttt{id} \mid \text{BLOCK} \mid \texttt{avg_pool} \\
\text{BLOCK} &::= \texttt{Linear3(ACT, CONV, NORM)} \\
\text{ACT} &::= \texttt{relu} \mid \texttt{hardswish} \mid \texttt{mish} \\
\text{CONV} &::= \texttt{conv1x1} \mid \texttt{conv3x3} \mid \texttt{dconv3x3} \\
\text{NORM} &::= \texttt{batch} \mid \texttt{instance} \mid \texttt{layer} \quad .
\end{aligned}
\tag{11}
$$

See Appendix A for the terminal vocabulary of topological operators and primitive computations. The productions with the nonterminals $\{\text{D2}, \text{D1}, \text{D0}, \text{D}\}$ define the spatial resolution flow and together with $\{\text{C}\}$ define the macro architecture containing possibly multiple branches. The productions for $\{\text{CL}, \text{OP}\}$ construct the NAS-Bench-201 cell and $\{\text{BLOCK}, \text{ACT}, \text{CONV}, \text{NORM}\}$ parameterize the convolutional block. To ensure that we use the same distribution over the primitive computations as in NAS-Bench-201, we reweigh the sampling probabilities of the productions generated by the nonterminal OP, i.e., all production choices have sampling probability of $20\,\%$, but BLOCK has $40\,\%$. Note that we omit the stem (i.e., 3x3 convolution followed by batch normalization) and classifier (i.e., batch normalization followed by ReLU, global average pooling, and fully-connected layer) for simplicity. We implemented the merge operation as element-wise summation. Different to the cell-based NAS-Bench-201 search space, we exclude degenerated architectures by introducing a constraint that ensures that each subterm maps the input to the output (i.e., in the associated computational graph there is at least one path from source to sink).

Our search space consists of ca. 10^{446} algebraic architecture terms (please refer to Appendix C on how to compute the search space size), which is significantly larger than other popular search spaces from the literature. For comparison, the cell-based NAS-Bench-201 search space is just a minuscule subspace of size $10^{4.18}$, where we apply only the blue-colored production rules and replace the CL nonterminals with a placeholder terminal x_1 that will be substituted by the searched, shared cell.

6.2 Evaluation Details

We compared four different search strategies, i.e., BANAT, Random Search (RS), Regularized Evolution (RE), and BANAT (WL) (Ru et al., 2021). For implementation details of the search strategies, please refer to Appendix G.1. We ran search for a total of 100 evaluations (including a random initial design of ten) on three seeds $\{777, 888, 999\}$ using 8 asynchronous workers each with a single NVIDIA RTX 2080 Ti GPU. In each evaluation, we fully trained the architecture candidate and recorded the last validation error.

We evaluated all search strategies on CIFAR-10/100 (Krizhevsky et al., 2009), ImageNet-16-120 (Chrabaszcz et al., 2017), CIFARTile, and AddNIST (Geada et al., 2021). We provide further dataset details in Appendix G.2. Note that CIFARTile and AddNIST are novel datasets and therefore have not yet been optimized by the research community. For training of architectures on CIFAR-10/100 and ImageNet-16-120, we followed Dong & Yang (2020). We trained architectures with SGD with learning rate of 0.1, Nesterov momentum of 0.9, weight decay of 0.0005 with cosine annealing (Loshchilov & Hutter, 2019), and batch size of 256 for 200 epochs. The initial channels were set to 16. For both CIFAR-10 and CIFAR-100, we used random flip with probability 0.5 followed by a random crop (32x32 with 4 pixel padding) and normalization. For ImageNet-16-120, we used a 16x16 random crop with 2 pixel padding instead. For training of architectures on AddNIST and CIFARTile, we followed the training protocol from the CVPR-NAS 2021 competition (Geada et al., 2021): We trained architectures with SGD with learning rate of 0.01, momentum of 0.9, and weight decay of 0.0003 with cosine annealing, and batch size of 64 for 64 epochs. We set the initial channels to 16 and did not apply any further data augmentation.

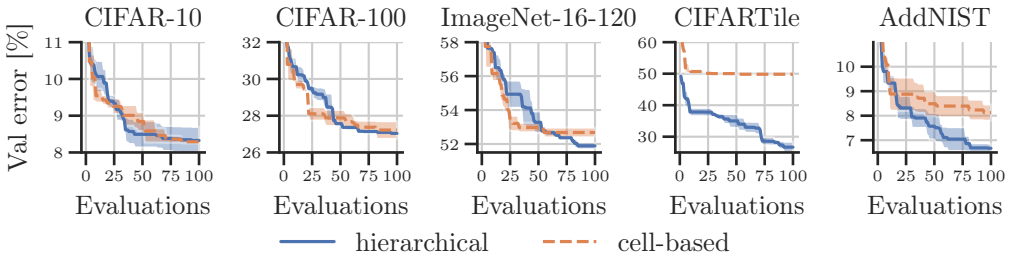

Figure 2: Cell-based vs. hierarchical search space. We plot mean and ± 1 standard error of the validation error on the cell-based (dashed orange) and hierarchical (solid blue) NAS-Bench-201 search space. We compare results using the other search strategies in Appendix G.3.

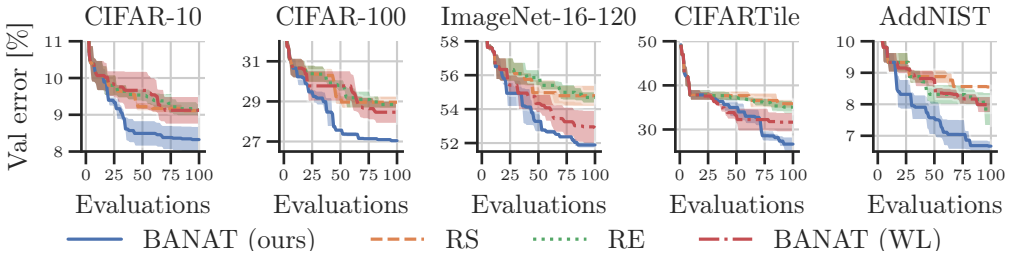

Figure 3: Comparison of search strategies on the hierarchical search space. We plot mean and ± 1 standard error of the validation error on the hierarchical NAS-Bench-201 search space for our search strategy BANAT (solid blue), RS (dashed orange), RE (dotted green), and BANAT (WL) (dash-dotted red). We report test errors, best architectures, and conduct further analyses in Appendix G.3.

To assess the modeling performance of our surrogate, we compared regression performance of a GP with our hierarchical WL kernel (hWL) against a GP with a WL kernel not leveraging the hierarchical information (WL) (Ru et al., 2021). We ran 20 trials over the seeds $\{0, 1, \ldots, 19\}$ and re-used the data from the search runs. In every trial, we sampled a training and test set of 700 or 500 architecture and validation error pairs, respectively. We fitted both surrogates with a varying number of training samples by randomly choosing samples from the training set without replacement, and recorded Spearman's rank and Pearson correlation between the predicted and true validation error.

6.3 Results

In the following we answer all of the questions **Q1**-**Q3**. Figure 2 compares the results of the cell-based and hierarchical search space design using our search strategy BANAT. Results with BANAT are on par on CIFAR-10/100, superior on ImageNet-16-120, and clearly superior on CIFARTile and AddNIST (answering **Q1**). We emphasize that the NAS community has engineered the cell-based search space to achieve strong performance on those popular image classification datasets for over a decade, making it unsurprising that our improvements are much larger for the novel datasets. Yet, our best found architecture on ImageNet-16-120 from the hierarchical search space also achieves an excellent test error of $52.78\,\%$ with only $0.626\,\mathrm{MB}$ parameters (Appendix G.3); this is superior to the state-of-the-art method Shapley-NAS (i.e., $53.15\,\%$) (Xiao et al., 2022) and on par with the *optimal* architecture of the cell-based NAS-Bench-201 search space (i.e., $52.69\,\%$ with $0.866\,\mathrm{MB}$). Figure 3 shows that our search strategy BANAT is also superior to common baselines (answering **Q2**) and that leveraging hierarchical information clearly improves performance (answering **Q3**). Further, the evaluation of surrogate performance in Figure 4 shows that incorporating hierarchical information with our hierarchical WL kernel (hWL) improves modeling, especially on smaller amounts of training data; this provides further evidence for answering **Q3**.

7 Discussion and Limitations

Our novel representation of neural architectures as algebraic terms could effectively represent any neural architecture. While this obviously does not imply that we can represent all neural architec-

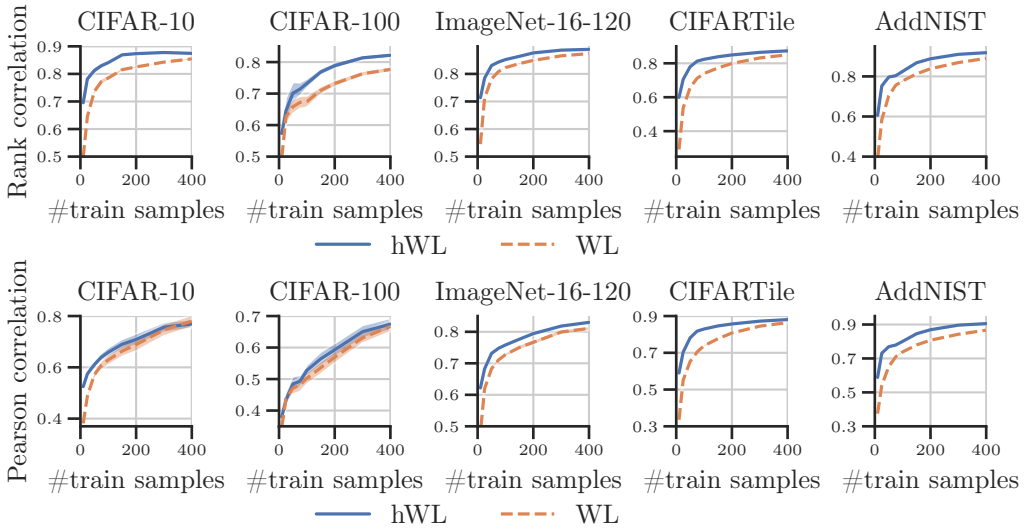

Figure 4: Mean Spearman's rank correlation (top) and Pearson correlation (bottom) with ± 1 standard error achieved by a GP with our hierarchical WL kernel (hWL) or without it (WL).

tures with a single search space based on our grammar-based approach from Section 3, our search spaces still significantly increase the expressiveness, including the ability to represent common search spaces from the literature (see Appendix E for how we can represent the search spaces of DARTS, Auto-Deeplab, the hierarchical cell search space of Liu et al. (2018), the Mobile-net search space, and the hierarchical random graph generator search space), as well as allowing search for entire neural architectures based around the popular NAS-Bench-201 search space (Section 6). Thus, our search space design can facilitate the discovery of novel well-performing neural architectures in those huge search spaces of algebraic architecture terms.

However, there is an inherent trade-off between the expressiveness and the difficulty of search. The much greater expressiveness facilitates search in a richer set of architectures that may include better architectures than in more restrictive search spaces, which however need not exist. Besides that, the (potential) existence of such a well-performing architecture does not result in a search strategy discovering it, even with large amounts of computing power available. Note that the trade-off manifests itself also in the acquisition function optimization of our search strategy BANAT.

In addition, a well-performing neural architecture may not work with current training protocols and hyperparameters due to interaction effects, i.e., training protocols and hyperparameters may be over-optimized for specific types of neural architectures. To overcome this limitation, one could consider a joint optimization of neural architectures, training protocols, and hyperparameters. However, this further fuels the trade-off between expressiveness and the difficulty of search.

Our grammar-based construction of search spaces of algebraic architecture terms also has its limitations. In particular, due to the discrete nature of CFGs we can not easily integrate continuous design choices, e.g., dropout probability. Furthermore, our grammar-based mechanism does not (generally) support simple scalability of discovered neural architectures (e.g., repetition of building blocks).

8 Conclusion

We introduced very expressive search spaces of algebraic architecture terms constructed with CFGs. To efficiently search over the huge search spaces, we proposed BANAT, an efficient BO strategy with a tailored kernel leveraging the available hierarchical information. Our experiments indicate that both our search space design and our search strategy can yield strong performance over existing baselines. Our results motivate further steps towards the discovery of neural architectures based on even more atomic primitive computations. Furthermore, future works could (simultaneously) learn the search space (i.e., learn the grammar) or improve search efficiency by means of multi-fidelity optimization or gradient-based search strategies.

REPRODUCIBILITY STATEMENT

To ensure reproducibility, we address all points of the best practices checklist for NAS research (Lindauer & Hutter, 2020) in Appendix H.

ETHICS STATEMENT

NAS has immense potential to facilitate systematic, automated discovery of high-performing (novel) architecture designs. However, the restrictive cell-based search spaces most commonly used in NAS render it impossible to discover truly novel neural architectures. With our general formalism based on algebraic terms, we hope to provide fertile foundation towards discovering high-performing and efficient architectures; potentially from scratch. However, search in such huge search spaces is expensive, particularly in the context of the ongoing detrimental climate crisis. While on the one hand, the discovered neural architectures, like other AI technologies, could potentially be exploited to have a negative societal impact; on the other hand, our work could also lead to advances across scientific disciplines like healthcare and chemistry.

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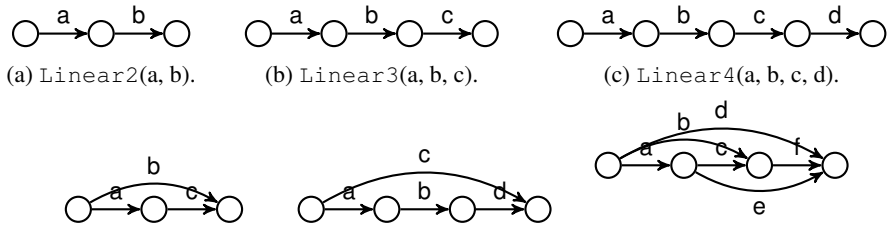
A FROM TERMINALS TO PRIMITIVE COMPUTATIONS AND TOPOLOGICAL OPERATORS

Table 1 and Figure 5 describe the primitive computations and topological operators used throughout our experiments in Section 6 and Appendix G, respectively. Note that by adding more primitive computations and/or topological operators we could construct even more expressive search spaces.

Table 1: Primitive computations. "Name" corresponds to the string terminals in our CFGs and "Function" is the associated implementation of the primitive computation in pseudocode. The subscripts g, k, s, and p are abbreviations for groups, kernel size, strides, and padding, respectively. During assembly of neural architectures $\Phi(\omega)$, we replace string terminals with the associated primitive computation.

Name	Function
`avg_pool`	$\texttt{AvgPool}_{k=3,s=1,p=1}\texttt{(x)}$
`batch`	`BN(x)`
`conv1x1`	$\texttt{Conv}_{k=1,s=1,p=0}(x)$
`conv3x3`	$\texttt{Conv}_{k=3,s=1,p=1}(x)$
`dconv3x3`	$\texttt{Conv}_{g=C,k=3,s=1,p=1}(x)$
`down`	$\texttt{conv3x3}_{s=1}\texttt{(conv3x3}_{s=2}\texttt{(x))} + \texttt{Conv}_{k=1,s=1}\texttt{(AvgPool}_{k=2,s=2}\texttt{(x))}$
`hardswish`	`Hardswish(x)`
`id`	`Identitiy(x)`
`instance`	`IN(x)`
`layer`	`LN(x)`
`mish`	`Mish(x)`
`relu`	`ReLU(x)`
`zero`	`Zeros(x)`



(a) `Linear2`(a, b). (b) `Linear3`(a, b, c). (c) `Linear4`(a, b, c, d).

(d) `Residual2`(a, b, c). (e) `Residual3`(a, b, c, d). (f) `Cell`(a, b, c, d, e, f).

Figure 5: Topological operators. Each subfigure makes the connection between the topogolocial operator and associated computational graph explicit, i.e., the arguments of the graph operators (a, b, ...) are mapped to the respective edges in the computational graph.

B EXTENDED BACKUS-NAUR FORM

The (extended) Backus-Naur form (Backus, 1959) is a meta-language to describe the syntax of CFGs. We use meta-rules of the form $\mathrm{S} ::= \alpha$ where $\mathrm{S} \in N$ is a nonterminal and $\alpha \in (N \cup \Sigma)^*$ is a string of nonterminals and/or terminals. We denote nonterminals in UPPER CASE, terminals corresponding to topological operators in `Initial upper case/teletype`, and terminals corresponding to primitive computations in `lower case/teletype`, e.g., $\mathrm{S} ::=$ `Residual`(S, S, `id`). To compactly express production rules with the same left-hand side nonterminal, we use the vertical bar | to indicate a choice of production rules with the same left-hand side, e.g., S ::= `Linear`(S, S, S) | `Residual`(S, S, `id`) | `conv`.

C SEARCH SPACE SIZE

In this section, we show how to efficiently compute the size of our search spaces constructed by CFGs. There are two cases to consider: (i) a CFG contains cycles (i.e., part of the derivation can be repeated infinitely many times) , yielding an open-ended, infinite search space; and (ii) a CFG contains no cycles, yielding in a finite search space whose size we can compute.

Consider a production $\mathrm{A} \rightarrow \texttt{Residual}(\mathrm{B},\ \mathrm{B},\ \mathrm{B})$ where `Residual` is a terminal, and A and B are nonterminals with $\mathrm{B} \rightarrow \texttt{conv} \mid \texttt{id}$. Consequently, there are $2^3 = 8$ possible instances of the residual block. If we add another production choice for the nonterminal A, e.g., $\mathrm{A} \rightarrow \texttt{Linear}(\mathrm{B},\ \mathrm{B},\ \mathrm{B})$, we would have $2^3 + 2^3 = 16$ possible instances. Further, adding a production $C \rightarrow \texttt{Linear}(\mathrm{A},\ \mathrm{A},\ \mathrm{A})$ would yield a search space size of $(2^3 + 2^3)^3 = 4096$.

More generally, we introduce the function P_{A} that returns the set of productions for nonterminal $\mathrm{A} \in N$, and the function $\mu : P \rightarrow N$ that returns all the nonterminals for a production $p \in P$. We can then recursively compute the size of the search space as follows:

$$f(\mathrm{A}) = \sum_{p \in P_{\mathrm{A}}} \begin{cases} 1 & ,\ \mu(p) = \emptyset, \\ \prod\limits_{\mathrm{A}' \in \mu(p)} f(\mathrm{A}') & ,\ otherwise \end{cases} . \tag{12}$$

When a CFG contains some constraint, we ensure to only account for valid architectures (i.e., compliant with the constraints) by ignoring productions which would lead to invalid architectures.

D MORE DETAILS ON SEARCH SPACE CONSTRAINTS

During the design of the search space, we may want to comply with some constraints, e.g., only consider valid neural architectures or impose structural constraints on architectures. We can guarantee compliance with constraints by modifying sampling (and evolution): we only allow the application of production rules, which guarantee compliance with the constraint(s). In the following, we show exemplary how this can be implemented for the former constraint mentioned above. Note that other constraints can be implemented in a similar manner

To implement the constraint "only consider valid neural architectures", we note that our search space design only creates neural architectures where neither the spatial resolution nor the channels can be mismatched; please refer to Section 3 for details. Thus, the only way a neural architecture can become invalid is through `zero` operations, which could remove edges from the computational graph and possibly disassociate the input from the output. Since we recursively assemble neural architectures, it is sufficient to ensure that the derived algebraic architecture term (i.e., the associated computational graph) is compliant with the constraint, i.e.,there is at least one path from input to output. Thus, during sampling (and similarly during evolution), we modify the current production rule choices when an application of the `zero` operation would disassociate the input from the output.

E COMMON SEARCH SPACES FROM THE LITERATURE

In Section 6.1, we demonstrated how to construct the popular NAS-Bench-201 search space within our algebraic search space design, and below we show how to reconstruct the following popular search spaces: DARTS search space (Liu et al., 2019b), Auto-DeepLab search space (Liu et al., 2019a), hierarchical cell search space (Liu et al., 2018), Mobile-net search space (Tan et al., 2019), and hierarchical random graph generator search space (Ru et al., 2020). For implementation details we refer to the respective works.

DARTS SEARCH SPACE

The DARTS search space (Liu et al., 2019b) consists of a fixed macro architecture and a cell, i.e., a seven node directed acyclic graph (`Darts`; see Figure 6 for the topological operator). We omit the fixed macro architecture from our search space design for simplicity. Each cell receives the feature maps from the two preceding cells as input and outputs a single feature map. All intermediate nodes

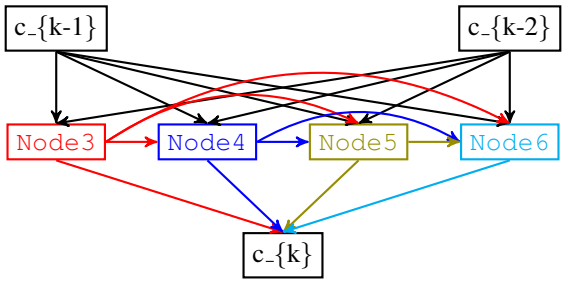


Figure 6: Visualization of the `Darts` topological operator.

(i.e., `Node3`, `Node4`, `Node5`, and `Node6`) is computed based on all of its predecessors. Thus, we can define the DARTS search space as follows:

$$
\begin{aligned}
\text{DARTS} &::= \texttt{Darts}(\text{NODE3, NODE4, NODE5, NODE6}) \\
\text{NODE3} &::= \texttt{Node3}(\text{OP, OP}) \\
\text{NODE4} &::= \texttt{Node4}(\text{OP, OP, OP}) \\
\text{NODE5} &::= \texttt{Node5}(\text{OP, OP, OP, OP}) \\
\text{NODE6} &::= \texttt{Node6}(\text{OP, OP, OP, OP, OP}) \\
\text{OP} &::= \texttt{sep_conv_3x3} \mid \texttt{sep_conv_5x5} \mid \texttt{dil_conv_3x3} \mid \texttt{dil_conv_5x5} \\
&\quad \mid \texttt{max_pool} \mid \texttt{avg_pool} \mid \texttt{id} \mid \texttt{zero} \quad ,
\end{aligned}
\tag{13}
$$

where the topological operator `Node3` receives two inputs, applies the operations separately on them, and sums them up. Similarly, `Node4`, `Node5`, and `Node6` apply their operations separately to the given inputs and sum them up. The topological operator `Darts` feeds the corresponding feature maps into each of those topological operators and finally concatenates all intermediate feature maps.

AUTO-DEEPLAB SEARCH SPACE

Auto-DeepLab (Liu et al., 2019a) combines a cell-level with a network-level search space to search for segmentation networks, where the cell is shared across the searched macro architecture, i.e., a twelve step (linear) path across different spatial resolutions. The cell-level design is adopted from Liu et al. (2019b) and, thus, we can re-use the CFG from Equation 13. For the network-level, we introduce a constraint that ensures that the path is of length twelve, i.e., we ensure exactly twelve derivations in our CFG. Further, we overload the nonterminals so that they correspond to the respective spatial resolution level, e.g., D4 indicates that the original input is downsampled by a factor of four; please refer to Section 3 for details on overloading nonterminals. For the sake of simplicity, we omit the first two layers and atrous spatial pyramid poolings as they are fixed, and hence define the network-level search space as follows:

$$
\begin{aligned}
\text{D4} &::= \texttt{Same}(\texttt{CELL}, \text{D4}) \mid \texttt{Down}(\texttt{CELL}, \textit{D8}) \\
\text{D8} &::= \texttt{Up}(\texttt{CELL}, \text{D4}) \mid \texttt{Same}(\texttt{CELL}, \text{D8}) \mid \texttt{Down}(\texttt{CELL}, \text{D16}) \\
\text{D16} &::= \texttt{Up}(\texttt{CELL}, \text{D8}) \mid \texttt{Same}(\texttt{CELL}, \text{D16}) \mid \texttt{Down}(\texttt{CELL}, \text{D32}) \\
\text{D32} &::= \texttt{Up}(\texttt{CELL}, \text{D16}) \mid \texttt{Same}(\texttt{CELL}, \text{D32}) \quad ,
\end{aligned}
\tag{14}
$$

where the topological operators `Up`, `Same`, and `Down` upsample/halve, do not change/do not change, or downsample/double the spatial resolution/channels, respectively. The placeholder variable `CELL` maps to the shared DARTS cell from the language generated by the CFG from Equation 13.

HIERARCHICAL CELL SEARCH SPACE

The hierarchical cell search space (Liu et al., 2018) consists of a fixed (linear) macro architecture and a hierarchically assembled cell with three levels which is shared across the macro architecture. Thus, we can omit the fixed macro architecture from our search space design for simplicity. Their first, second, and third hierarchical levels correspond to the primitive computations (i.e., `id`, `max_pool`, `avg_pool`, `sep_conv`, `depth_conv`, `conv`, `zero`), six densely connected four node directed acyclic graphs (`DAG4`), and a densely connected five node directed acyclic graph (`DAG5`), respectively. The `zero` operation could lead to directed acyclic graphs which have fewer nodes. Therefore,

we introduce a constraint enforcing that there are always four (level 2) or five (level 3) nodes for every directed acyclic graph. Further, since a densely connected five node directed acyclic graph graph has ten edges, we need to introduce placeholder variables (i.e., `M1`, ..., `M6`) to enforce that only six (possibly) different four node directed acyclic graphs are used, and consequently define a CFG for the third level

$$\begin{aligned} \text{LEVEL3} &::= \texttt{DAG5}(\underbrace{\text{LEVEL2, ..., LEVEL2}}_{\times 10}) \\ \text{LEVEL2} &::= \texttt{M1} \mid \texttt{M2} \mid \texttt{M3} \mid \texttt{M4} \mid \texttt{M5} \mid \texttt{M6} \mid \texttt{zero} \quad , \end{aligned} \tag{15}$$

mapping the placeholder variables `M1`, ..., `M6` to the six lower-level motifs constructed by the first and second hierarchical level

$$\begin{aligned} \text{LEVEL2} &::= \texttt{DAG4}(\underbrace{\text{LEVEL1, ..., LEVEL1}}_{\times 6}) \\ \text{LEVEL1} &::= \texttt{id} \mid \texttt{max_pool} \mid \texttt{avg_pool} \mid \texttt{sep_conv} \mid \texttt{depth_conv} \mid \texttt{conv} \mid \texttt{zero} \quad . \end{aligned} \tag{16}$$

MOBILE-NET SEARCH SPACE

Factorized hierarchical search spaces, e.g., the Mobile-net search space (Tan et al., 2019), allow for layer diversity. They factorize a (fixed) macro architecture – often based on an already well-performing reference architecture – into separate blocks (e.g., cells). For the sake of simplicity, we assume here a three sequential blocks (`Block`) architecture (`Linear`). In each of those blocks, we search for the convolution operations (CONV), kernel sizes (KSIZE), squeeze-and-excitation ratio (SERATIO) (Hu et al., 2018), skip connections (SKIP), number of output channels (FSIZE), and number of layers per block (#LAYERS), where the latter two are discretized using a reference architecture, e.g., MobileNetV2 (Sandler et al., 2018). Consequently, we can express this search space as follows:

$$\begin{aligned} \text{MACRO} &::= \texttt{Linear}(\text{BLOCK, BLOCK, BLOCK}) \\ \text{BLOCK} &::= \texttt{Block}(\text{CONV, KSIZE, SERATIO, SKIP, FSIZE, \#LAYERS}) \\ \text{CONV} &::= \texttt{conv} \mid \texttt{dconv} \mid \texttt{mbconv} \\ \text{KSIZE} &::= \texttt{3} \mid \texttt{5} \\ \text{SERATIO} &::= \texttt{0} \mid \texttt{0.25} \\ \text{SKIP} &::= \texttt{pooling} \mid \texttt{id_residual} \mid \texttt{no_skip} \\ \text{FSIZE} &::= \texttt{0.75} \mid \texttt{1.0} \mid \texttt{1.25} \\ \text{\#LAYERS} &::= \texttt{-1} \mid \texttt{0} \mid \texttt{1} \quad , \end{aligned} \tag{17}$$

where `conv`, `donv` and `mbconv` correspond to convolution, depthwise convolution, and mobile inverted bottleneck convolution (Sandler et al., 2018), respectively.

HIERARCHICAL RANDOM GRAPH GENERATOR SEARCH SPACE

The hierarchical random graph generator search space (Ru et al., 2020) consists of three hierarchical levels of random graph generators (i.e., `Watts-Strogatz` (Watts & Strogatz, 1998) and `Erdõs-Rényi` (Erdős et al., 1960)). We denote with `Watts-Strogatz_i` the random graph generated by the Watts-Strogatz model with i nodes. Thus, we can represent the search space as follows:

$$\begin{aligned} \text{TOP} &::= \texttt{Watts-Strogatz_3}(\text{K, }\texttt{Pt})(\text{MID, MID, MID}) \mid ... \\ &\quad \mid \texttt{Watts-Strogatz_10}(\text{K, }\texttt{Pt})(\underbrace{\text{MID, ..., MID}}_{\times 10}) \\ \text{MID} &::= \texttt{Erdõs-Rényi_1}(\texttt{Pm})(\text{BOT}) \mid ... \\ &\quad \mid \texttt{Erdõs-Rényi_10}(\texttt{Pm})(\underbrace{\text{BOT, ..., BOT}}_{\times 10}) \\ \text{BOT} &::= \texttt{Watts-Strogatz_3}(\text{K, }\texttt{Pb})(\texttt{NODE, NODE, NODE}) \mid ... \\ &\quad \mid \texttt{Watts-Strogatz_10}(\text{K, }\texttt{Pb})(\underbrace{\texttt{NODE ..., NODE}}_{\times 10}) \\ \text{K} &::= \texttt{2} \mid \texttt{3} \mid \texttt{4} \mid \texttt{5} \quad , \end{aligned} \tag{18}$$

Algorithm 1 Bayesian Optimization algorithm (Brochu et al., 2010).

Input: Initial observed data $\mathcal{D}_t$, a black-box objective function f, total number of BO iterations T
Output: The best recommendation about the global optimizer $\mathbf{x}^*$
for $t = 1, \ldots, T$ **do**
  Select the next $\mathbf{x}_{t+1}$ by maximizing acquisition function $\alpha(\mathbf{x}|\mathcal{D}_t)$
  Evaluate the objective function at $f_{t+1} = f(\mathbf{x}_{t+1})$
  $\mathcal{D}_{t+1} \leftarrow \mathcal{D}_t \cup (\mathbf{x}_{t+1}, f_{t+1})$
  Update the surrogate model with $\mathcal{D}_{t+1}$
end for

where each terminal `Pt`, `Pm`, and `Pb` maps to a continuous number in $[0.1,\ 0.9]$[1] and the placeholder variable `NODE` maps to a primitive computation, e.g., separable convolution. Note that we omit other hyperparameters, such as stage ratio, channel ratio etc., for simplicity.

F MORE DETAILS ON THE SEARCH STRATEGY

In this section, we provide more details and examples for our search strategy Bayesian Optimization for Algebraic Neural Architecture Terms (BANAT) presented in Section 4.

F.1 BAYESIAN OPTIMIZATION

Bayesian Optimization (BO) is a powerful family of search techniques for finding the global optimum of a black-box objective problem. It is particularly useful when the objective is expensive to evaluate and thus sample efficiency is highly important (Brochu et al., 2010).

To minimize a black-box objective problem with BO, we first need to build a probabilistic surrogate to model the objective based on the observed data so far. Based on the surrogate model, we design an acquisition function to evaluate the utility of potential candidate points by trading off exploitation (where the posterior mean of the surrogate model is low) and exploration (where the posterior variance of the surrogate model is high). The next candidate points to evaluate is then selected by maximizing the acquisition function (Shahriari et al., 2015). The general procedures of BO is summarized in Algorithm 1.

We adopted the widely used acquisition function, expected improvement (EI) (Mockus et al., 1978), in our BO strategy. EI evaluates the expected amount of improvement of a candidate point $\mathbf{x}$ over the minimal value f' observed so far. Specifically, denote the improvement function as $I(\mathbf{x}) = \max(0, f' - f(\mathbf{x}))$, the EI acquisition function has the form

$$\begin{aligned}\alpha_{EI}(\mathbf{x}|\mathcal{D}_t) = \mathbb{E}[I(\mathbf{x})|\mathcal{D}_t] &= \int_{-\infty}^{f'} (f' - f)\mathcal{N}\left(f; \mu(\mathbf{x}|\mathcal{D}_t), \sigma^2(\mathbf{x}|\mathcal{D}_t)\right) df \\ &= (f' - f)\Phi\left(f'; \mu(\mathbf{x}|\mathcal{D}_t), \sigma^2(\mathbf{x}|\mathcal{D}_t)\right) + \sigma^2(\mathbf{x}|\mathcal{D}_t)\phi(f'; \mu(\mathbf{x}|\mathcal{D}_t), \sigma^2(\mathbf{x}|\mathcal{D}_t)) \quad ,\end{aligned}$$

where $\mu(\mathbf{x}|\mathcal{D}_t)$ and $\sigma^2(\mathbf{x}|\mathcal{D}_t)$ are the mean and variance of the predictive posterior distribution at a candidate point $\mathbf{x}$, and $\phi(\cdot)$ and $\Phi(\cdot)$ denote the PDF and CDF of the standard normal distribution, respectively.

To make use of ample distributed computing resource, we adopted Kriging Believer (Ginsbourger et al., 2010) which uses the predictive posterior of the surrogate model to assign hallucinated function values $\{\tilde{f}_p\}_{p \in \{1,\ \ldots,\ P\}}$ to the P candidate points with pending evaluations $\{\tilde{\mathbf{x}}_p\}_{p \in \{1,\ \ldots,\ P\}}$ and perform next BO recommendation in the batch by pseudo-augmenting the observation data with $\tilde{\mathcal{D}}_p = \{(\tilde{\mathbf{x}}_p, \tilde{f}_p)\}_{p \in \{1,\ \ldots,\ P\}}$, namely $\tilde{\mathcal{D}}_t = \mathcal{D}_t \cup \tilde{\mathcal{D}}_p$. The algorithm of Kriging Believer at one BO iteration to select a batch of recommended candidate points is summarized in Algorithm 2.

[1] Theoretically, this is not possible with CFGs. However, we can extend the notion of substitution by substituting a string representation of a Python (float) variable for the placeholder variables `Pt`, `Pm`, and `Pb`.

Algorithm 2 Kriging Believer algorithm to select one batch of points.

Input: Observation data $\mathcal{D}_t$, batch size b
Output: The batch points $\mathcal{B}_{t+1} = \{\mathbf{x}_{t+1}^{(1)}, \ldots, \mathbf{x}_{t+1}^{(b)}\}$
$\tilde{\mathcal{D}}_t = \mathcal{D}_t \cup \tilde{\mathcal{D}}_p$
for $j = 1, \ldots, b$ **do**
  Select the next $\mathbf{x}_{t+1}^{(j)}$ by maximizing acquisition function $\alpha(\mathbf{x}|\tilde{\mathcal{D}}_t)$
  Compute the predictive posterior mean $\mu(\mathbf{x}_{t+1}^{(j)}|\tilde{\mathcal{D}}_t)$
  $\tilde{\mathcal{D}}_t \leftarrow \tilde{\mathcal{D}}_t \cup (\mathbf{x}_{t+1}, \mu(\mathbf{x}_{t+1}^{(j)}|\tilde{\mathcal{D}}_t))$
end for

Algorithm 3 Weisfeiler-Lehman subtree kernel computation (Shervashidze et al., 2011).

Input: Graphs G_1, G_2, maximum iterations H
Output: Kernel function value between the graphs
Initialize the feature vectors $\phi(G_1) = \phi_0(G_1), \phi(G_2) = \phi_0(G_2)$ with the respective counts of original node labels (i.e., the $h = 0$ WL features)
for $h = 1, \ldots H$ **do**
  Assign a multiset $M_h(v) = \{l_{h-1}(u) | u \in \mathcal{N}(v)\}$ to each node $v \in G$, where l_{h-1} is the node label function of the $h-1$-th WL iteration and $\mathcal{N}$ is the node neighbor function
  Sort elements in multiset $M_h(v)$ and concatenate them to string $s_h(v)$
  Compress each string $s_h(v)$ using the hash function f s.t. $f(s_h(v)) = f(s_h(w)) \iff s_h(v) = s_h(u)$
  Add l_{h-1} as prefix for $s_h(v)$
  Concatenate the WL features $\phi_h(G_1), \phi_h(G_2)$ with the respective counts of the *new* labels: $\phi(G_1) = [\phi(G_1), \phi_h(G_1)], \phi(G_2) = [\phi(G_2), \phi_h(G_2)]$
  Set $l_h(v) := f(s_h(v)) \; \forall v \in G$
end for
Compute inner product $k = \langle \phi_h(G_1), \phi_h(G_2) \rangle$ between WL features $\phi_h(G_1), \phi_h(G_2)$ in RKHS $\mathcal{H}$

F.2 Weisfeiler-Lehman kernel

Inspired by Ru et al. (2021), we adopted the Weisfeiler-Lehman (WL) graph kernel (Shervashidze et al., 2011) in the GP surrogate model to handle the graph nature of neural architectures. The basic idea of the WL kernel is to first compare node labels, and then iteratively aggregate labels of neighboring nodes, compress them into a new label and compare them. Algorithm 3 summarizes the WL kernel procedure.

Ru et al. (2021) identified three reasons for using the WL kernel: (1) it is able to compare labeled and directed graphs of different sizes, (2) it is expressive, and (3) it is relatively efficient and scalable. Our search space design can afford a diverse spectrum of neural architectures with very heterogeneous topological structure. Therefore, reason (1) is a very important property of the WL kernel to account for the diversity of neural architectures. Moreover, if we allow many hierarchical levels, we can construct very large neural architectures. Therefore, reasons (2) and (3) are essential for accurate and fast modeling. However, neural architectures in our search spaces may be significantly larger, which makes it difficult for a single WL kernel to capture the more global topological patterns. Moreover, modeling solely based on the final neural architecture ignores the useful macro-level information from earlier hierarchical levels. In our experiments (Section 6 and G), we have found stronger neural architectures by incorporating the hierarchical information in the kernel design, which provides experimental support for above arguments.

F.3 Examples for the evolutionary operations

For the evolutionary operations, we adopted ideas from grammar-based genetic programming (McKay et al., 2010; Moss et al., 2020). In the following, we will show how these evolutionary operations manipulate algebraic terms, e.g.,

$$\texttt{Linear(Residual(conv, id, conv), Residual(conv, id, conv), fc)} \quad , \tag{19}$$

Table 2: Licenses for the datasets we used in our experiments.

Dataset	License	URL
CIFAR-10 (Krizhevsky et al., 2009)	MIT	https://www.cs.toronto.edu/~kriz/cifar.html
CIFAR-100 (Krizhevsky et al., 2009)	MIT	https://www.cs.toronto.edu/~kriz/cifar.html
ImageNet-16-120 (Chrabaszcz et al., 2017)	MIT	https://patrykchrabaszcz.github.io/Imagenet32/
CIFARTile (Geada et al., 2021)	GNU	https://github.com/RobGeada/cvpr-nas-datasets
AddNIST (Geada et al., 2021)	GNU	https://github.com/RobGeada/cvpr-nas-datasets

from the search space

$$\mathrm{S} \ ::= \ \texttt{Linear}(\mathrm{S},\ \mathrm{S},\ \mathrm{S}) \mid \texttt{Residual}(\mathrm{S},\ \mathrm{S},\ \mathrm{S}) \mid \texttt{conv} \mid \texttt{id} \mid \texttt{fc} \quad , \tag{20}$$

to generate evolved algebraic terms. Figure 1 shows how we can derive the algebraic term in Equation 19 from the search space in Equation 20. For mutation operations, we first randomly pick a subterm of the algebraic term, e.g., `Residual(conv, id, conv)`. Then, we randomly sample a new subterm with the same nonterminal symbol S as start symbol, e.g., `Linear(conv, id, fc)`, and replace the previous subterm, yielding

$$\texttt{Linear}(\texttt{Linear}(\texttt{conv},\ \texttt{id},\ \texttt{fc}),\ \texttt{Residual}(\texttt{conv},\ \texttt{id},\ \texttt{conv}),\ \texttt{fc}) \quad . \tag{21}$$

For (self-)crossover operations, we swap two subterms, e.g., `Residual(conv, id, conv)` and `Residual(conv, id, conv)` with the same nonterminal S as start symbol, yielding

$$\texttt{Linear}(\texttt{Residual}(\texttt{conv},\ \texttt{id},\ \texttt{conv}),\ \texttt{Residual}(\texttt{conv},\ \texttt{id},\ \texttt{conv}),\ \texttt{fc}) \quad . \tag{22}$$

Note that unlike the commonly used crossover operation, which uses two parents, self-crossover has only one parent. In future work, we could also add a *self-copy* operation that copies a subterm to another part of the algebraic term, explicitly regularizing diversity and thus potentially speeding up the search.

G Details for Section 6

In this section, we report implementation details (Section G.1) as well as dataset details (Section G.2). We also present the search results and conduct an analyses on the architectures observed during all of our search runs (Section G.3).

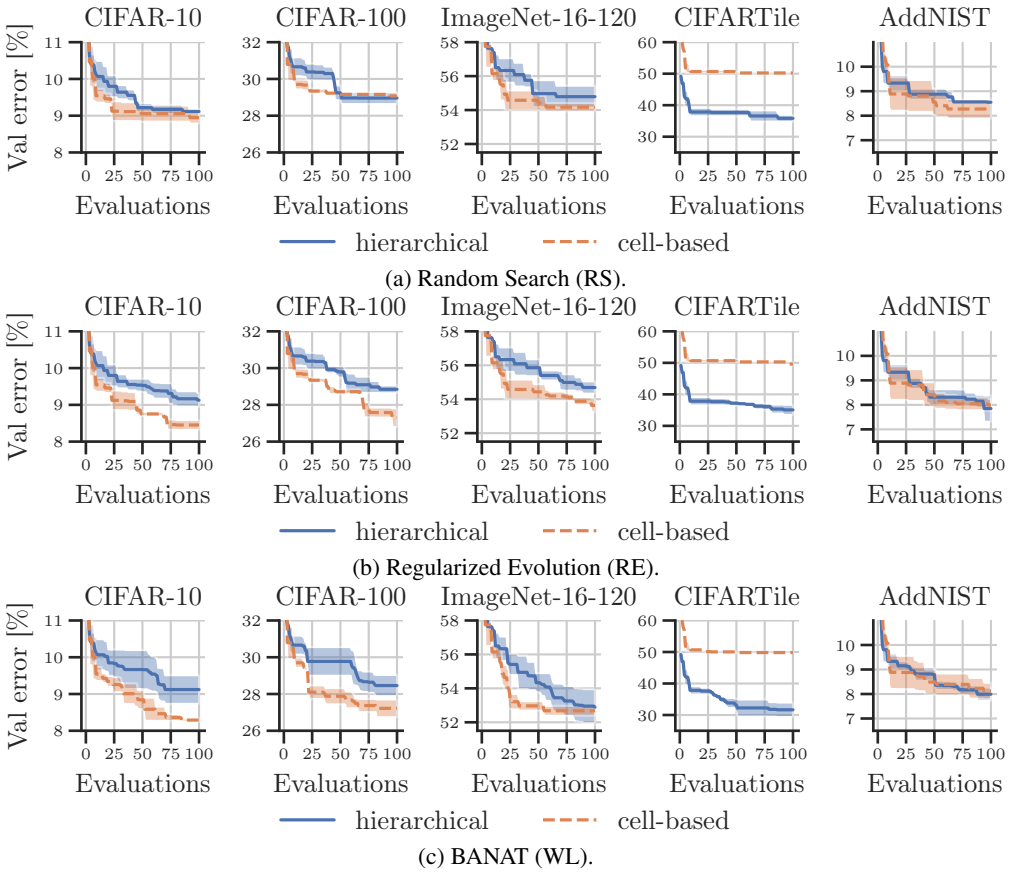
G.1 Implementation details

BANAT & BANAT (WL) The only difference between BANAT and BANAT (WL) is that the former uses our proposed hierarchy of WL kernels (hWL), whereas the latter only uses a single WL kernel (WL) for the entire architecture (c.f., (Ru et al., 2021)). We ran BANAT asynchronously in parallel throughout our experiments with a batch size of $B = 1$, i.e., at each BO iteration a single architecture is proposed for evaluation. For the evolutionary acquisition function optimization, we used a pool size of $P = 200$, where the initial population consisted of the current ten best-performing architectures and the remainder were randomly sampled architectures to encourage exploration in the huge search spaces. During evolution, the mutation probability was set to $p_{mut} = 0.5$ and crossover probability was set to $p_{cross} = 0.5$. From the crossovers, half of them were self-crossovers of one parent and the other half were common crossovers between two parents. The tournament selection probability was set to $p_{tour} = 0.2$. We evolved the population at least for ten iterations and a maximum of 50 iterations using a early stopping criterion based on the fitness value improvements over the last five iterations.

Regularized Evolution (RE) RE iteratively mutates the best architectures out of a sample of the population. We reduced the population size from 50 to 30 to account for fewer evaluations, and used a sample size of 10. We also ran RE asynchronously for better comparability.

G.2 Dataset details

In Table 2, we provide the licenses for the datasets used in our experiments. For training of architectures on CIFAR-10, CIFAR-100 (Krizhevsky et al., 2009), and ImageNet-16-120 (Chrabaszcz



(a) Random Search (RS).

(b) Regularized Evolution (RE).

(c) BANAT (WL).

Figure 7: Cell-based vs. hierarchical search spaces. We plot mean and ± 1 standard error of the validation error on the cell-based (dashed orange) and hierarchical (solid blue) NAS-Bench-201 search space using Random Search (RS) (top), Regularized Evolution (RE) (middle), and BANAT (WL) (bottom).

et al., 2017), we followed the dataset splits and training protocol of NAS-Bench-201 (Dong & Yang, 2020). For CIFAR-10, we split the original training set into a new training set with 25k images and validation set with 25k images following Dong & Yang (2020). The test set remained unchanged. For evaluation, we trained architectures on both the training and validation set. For CIFAR-100, the training set remained unchanged, but the test set was partitioned in a validation set and new test set with each 5K images. For ImageNet-16-120, all splits remained unchanged. For AddNIST and CIFARTile, we used the training, validation, and test splits as defined in the CVPR-NAS 2021 competition (Geada et al., 2021).

G.3 Further search results and analyses

Supplementary to Figure 2, Figure 7 compares the cell-based vs. hierarchical NAS-Bench-201 search space from Section 6.1 using RS, RE, and BANAT (WL). The cell-based search space design shows on par or stronger performance on all datasets except for CIFARTile for the three search strategies. In contrast, for our proposed search strategy BANAT we find on par (CIFAR-10/100) or superior (ImageNet-16-120, CIFARTile, and AddNIST) performance using the hierarchical search space design. This clearly shows that the increase of the search space does not necessarily yields the discovery of stronger neural architectures. Further, it exemplifies the importance of a strong search strategy to search effectively and efficiently in huge hierarchical search spaces (**Q2**), and provides further evidence that the incorporation of hierarchical information is a key contributor for search efficiency (**Q3**). Based on this, we believe that future work using, e.g., graph neural networks as a surrogate, may benefit from the incorporation of hierarchical information.

Table 3: Test errors (and ± 1 standard error) of popular baseline architectures (e.g., ResNet (He et al., 2016) and EfficientNet (Tan & Le, 2019) variants), and our best found architectures on the cell-based and hierarchical NAS-Bench-201 search space. Note that we picked the ResNet and EfficientNet variant based on the test error, consequently giving an overestimate of their test performance.
† optimal numbers as reported in Dong & Yang (2020).
(val best) test error (and ± 1 standard error) across three seeds $\{777,\ 888,\ 999\}$ of the best architecture of the three search runs with lowest validation error.

Method	CIFAR-10		CIFAR-100		ImageNet-16-120		CIFARTile		AddNIST	
	cell-based	hierarchical	cell-based	hierarchical	cell-based	hierarchical	cell-based	hierarchical	cell-based	hierarchical
Best ResNet (He et al., 2016)	6.49 $\pm$ 0.24 (32)		27.1 $\pm$ 0.67 (110)		53.67 $\pm$ 0.18 (56)		57.8 $\pm$ 0.57 (18)		7.78 $\pm$ 0.05 (34)	
Best EfficientNet (Tan & Le, 2019)	11.73 $\pm$ 0.1 (B0)		35.17 $\pm$ 0.42 (B6)		77.73 $\pm$ 0.29 (B0)		61.01 $\pm$ 0.62 (B0)		13.24 $\pm$ 0.58 (B1)	
NAS-Bench-201 oracle†	5.63		26.49		52.69		-		-	
RS	6.39 $\pm$ 0.18	6.77 $\pm$ 0.1	28.75 $\pm$ 0.57	29.49 $\pm$ 0.57	54.83 $\pm$ 0.78	54.7 $\pm$ 0.82	**52.72 $\pm$ 0.45**	40.93 $\pm$ 0.81	7.82 $\pm$ 0.36	8.05 $\pm$ 0.29
RE	**5.76 $\pm$ 0.17**	6.88 $\pm$ 0.24	27.68 $\pm$ 0.55	30.0 $\pm$ 0.32	53.92 $\pm$ 0.6	55.39 $\pm$ 0.54	52.79 $\pm$ 0.59	40.99 $\pm$ 2.89	**7.69 $\pm$ 0.35**	7.56 $\pm$ 0.69
BANAT (WL)	**5.68 $\pm$ 0.11**	6.98 $\pm$ 0.5	27.66 $\pm$ 0.18	28.7 $\pm$ 0.64	53.67 $\pm$ 0.39	53.47 $\pm$ 0.86	52.81 $\pm$ 0.27	35.75 $\pm$ 1.58	7.86 $\pm$ 0.41	8.2 $\pm$ 0.37
BANAT	**5.68 $\pm$ 0.11**	**6.0 $\pm$ 0.16**	27.66 $\pm$ 0.18	27.57 $\pm$ 0.46	53.67 $\pm$ 0.39	53.43 $\pm$ 0.61	52.81 $\pm$ 0.27	**32.28 $\pm$ 2.39**	7.86 $\pm$ 0.41	**6.09 $\pm$ 0.34**
BANAT (best)	5.64 $\pm$ 0.14	5.65 $\pm$ 0.09	27.03 $\pm$ 0.23	27.63 $\pm$ 0.2	53.54 $\pm$ 0.43	52.78 $\pm$ 0.23	53.18 $\pm$ 0.91	30.33 $\pm$ 0.77	8.04 $\pm$ 0.45	6.33 $\pm$ 0.59

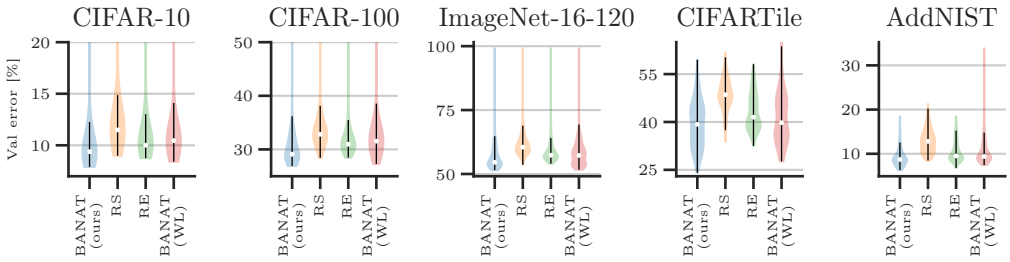


Figure 8: Density estimates for the validation error of all architecture candidates proposed by the search strategies (i.e., BANAT, RS, RE, and BANAT (WL)) and across datasets (i.e., CIFAR-10/100, ImageNet-16-120, CIFARTile, AddNIST) from our experiments in Section 6.

We report the test errors of our best found architectures in Table 3. We observe that our search strategy BANAT finds the strongest performing architectures across all dataset (**Q2**, **Q3**). Also note that we achieve better (validation and) test performance on ImageNet-16-120 on the hierarchical than the state-of-the-art search strategy on the cell-based NAS-Bench-201 search space (i.e., $+0.37\%p$ compared to Shapley-NAS (Xiao et al., 2022)) (**Q1**).

Search costs Search time varied across datasets from ca. 0.5 days (CIFAR-10) to ca. 1.8 days (ImageNet-16-120) using eight asynchronous workers, each with an NVIDIA RTX 2080 Ti GPU.

Is our search strategy BANAT exploring well-performing architectures during search? To investigate the question, we studied density estimates of the validation error of proposed candidates for all search strategies across our experiments from Section 6. This provides a better view for whether search strategies are exploring well-performing architectures or wasting computational resources on low-performing architectures. Figure 8 shows that our proposed search strategy BANAT explored better architecture candidates across all the datasets, i.e., it has smaller median validation errors and the distributions are further shifted towards smaller validation errors than for the other search strategies.

What distinguishes top-performing neural architectures from the other ones? To understand what distinguishes top-performing neural architecture from other ones, we analyze the impact of maximum depth on performance and the frequency of production rules in the worst-10%, top-10%, or other neural architectures, respectively. In another analysis, we marginalize out the validation error of every production rule; thereby relating the contribution of a production rule with the performance of the architecture. Note, however, that both analyses ignore the topological information, i.e., a topological operator or primitive computation may have a different effect at different stages of the architecture.

Figure 9 shows no particular trend (e.g., more depth yields better performance) across the datasets, indicating that depth may not be the most important factor for performance in our hierarchical search space. In contrast, Figure 10 and Figure 11 show that particularly macro-level production rules (i.e., for the nonterminals D2, D1, D0, and D) have a large effect on the performance of an architecture. Interestingly, we find that that top-performing architectures (almost exclusively) use the topological operator `Residual3` for derivations from the nonterminal D1 across search spaces. This hints that a residual connection at the macro-level could be a strong topological structure, but remains to be evaluated for a variety of architectures. Cell-level production choices have less effect on performance. However, we hypothesize that this may also be due to the neglect of topological information. We leave further analysis for future work.

Best architectures Below we report the best found architecture per dataset on the hierarchical NAS-Bench-201 search space (Section 6.1) for each dataset. Figure 12 provides a graphical summary of the best architectures.

CIFAR-10 (mean test error $5.65\,\%$, #params $2.204\,\mathrm{MB}$, FLOPs $127.673\,\mathrm{M}$):

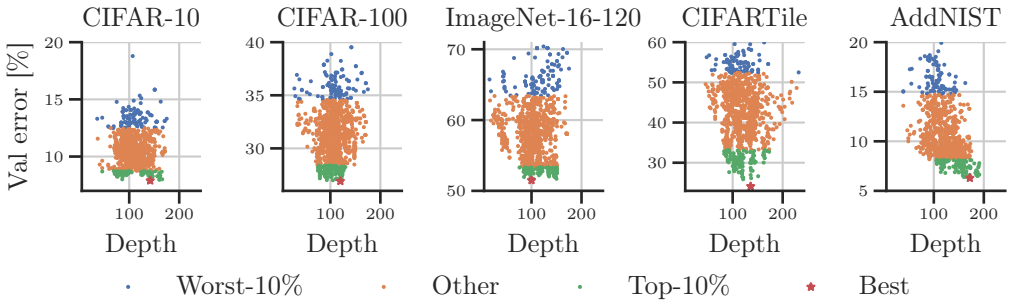
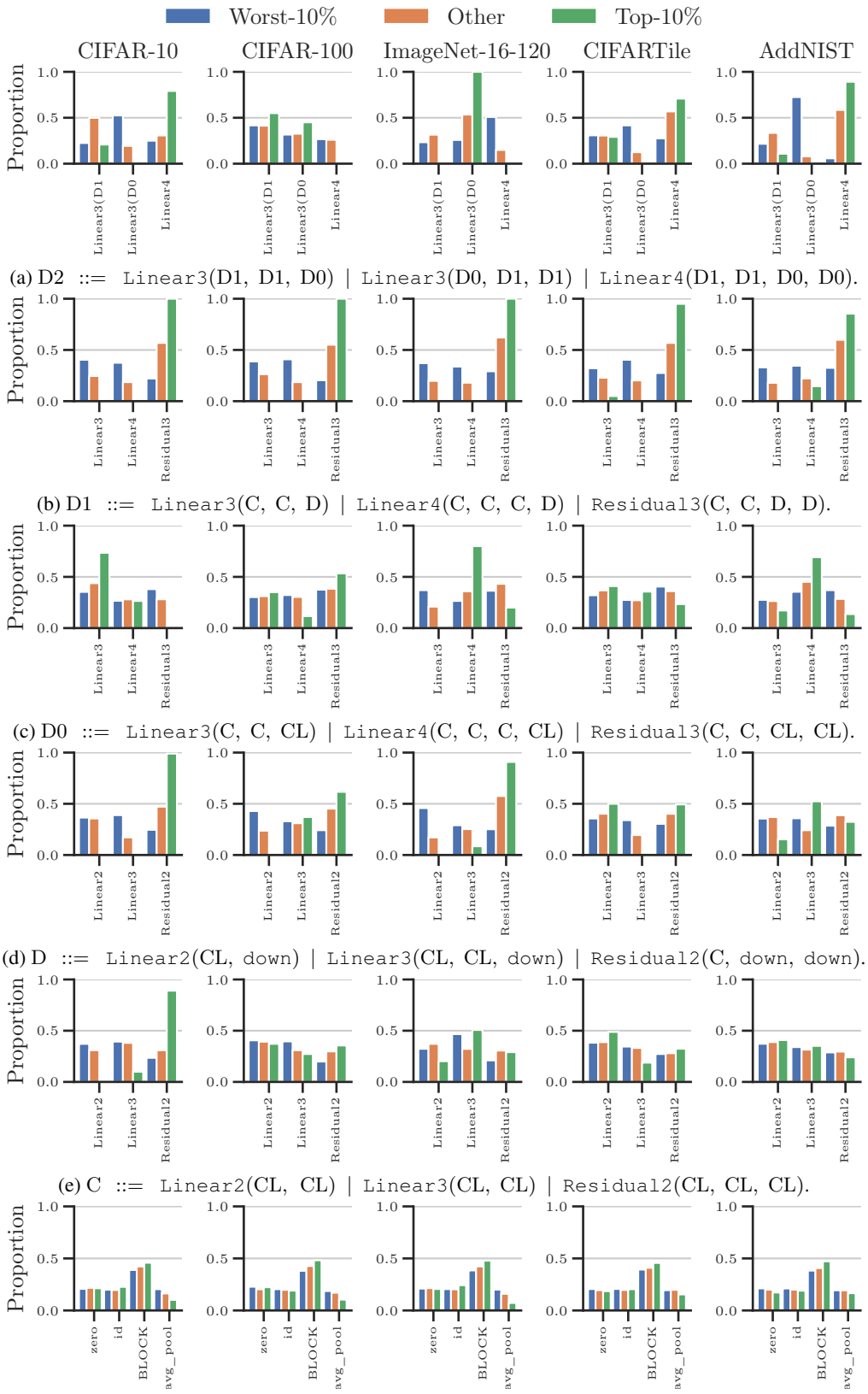


Figure 9: Validation error over maximal depth of all architecture candidates proposed by the search strategies (i.e., BANAT, RS, RE, and BANAT (WL)) and across datasets (i.e., CIFAR-10/100, ImageNet-16-120, CIFARTile, AddNIST) from our experiments in Section 6.

Linear4(Residual3(Residual2(Cell(id, zero, Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(hardswish, conv3x3, layer)), zero, Linear1(Linear3(mish, conv3x3, instance))), Cell(Linear1(Linear3(relu, dconv3x3, layer)), id, avg_pool, Linear1(Linear3(relu, dconv3x3, layer)), id, zero), Cell(zero, Linear1(Linear3(relu, conv1x1, layer)), id, Linear1(Linear3(hardswish, conv1x1, instance)), Linear1(Linear3(hardswish, conv3x3, layer)), Linear1(Linear3(hardswish, dconv3x3, layer)))), Residual2(Cell(id, zero, Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(mish, conv1x1, layer)), Linear1(Linear3(hardswish, conv3x3, layer)), zero), Cell(id, zero, id, Linear1(Linear3(relu, conv3x3, batch)), id, id), Cell(Linear1(Linear3(hardswish, conv3x3, layer)), Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv3x3, layer)), zero, id)), Residual2(Cell(Linear1(Linear3(hardswish, conv1x1, instance)), Linear1(Linear3(hardswish, dconv3x3, batch)), Linear1(Linear3(mish, dconv3x3, instance)), Linear1(Linear3(relu, conv1x1, batch)), id, id), down, down), Residual2(Cell(Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(hardswish, dconv3x3, batch)), Linear1(Linear3(relu, conv1x1, batch)), Linear1(Linear3(hardswish, conv3x3, layer)), id, avg_pool), down, down)), Residual3(Residual2(Cell(id, zero, Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(hardswish, conv3x3, layer)), id, Linear1(Linear3(mish, conv3x3, instance))), Cell(Linear1(Linear3(relu, dconv3x3, layer)), id, avg_pool, Linear1(Linear3(relu, dconv3x3, layer)), id, zero), Cell(zero, Linear1(Linear3(relu, conv1x1, layer)), id, Linear1(Linear3(hardswish, conv1x1, instance)), Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(hardswish, dconv3x3, layer)))), Residual2(Cell(id, zero, Linear1(Linear3(mish, conv1x1, layer)), Linear1(Linear3(mish, conv3x3, layer)), Linear1(Linear3(hardswish, dconv3x3, batch)), zero), Cell(id, zero, id, Linear1(Linear3(relu, conv3x3, batch)), id, id), Cell(Linear1(Linear3(hardswish, conv3x3, layer)), Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(mish, conv1x1, batch)), Linear1(Linear3(relu, conv3x3, instance)), zero, id)), Residual2(Cell(Linear1(Linear3(relu, conv1x1, batch)), Linear1(Linear3(hardswish, dconv3x3, batch)), id, Linear1(Linear3(relu, conv1x1, batch)), id, id), down, down), Residual2(Cell(Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(hardswish, dconv3x3, batch)), Linear1(Linear3(relu, conv1x1, batch)), Linear1(Linear3(hardswish, conv3x3, layer)), id, avg_pool), down, down)), Linear3(Residual2(Cell(Linear1(Linear3(hardswish, conv3x3, batch)), Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv1x1, layer)), id), Cell(Linear1(Linear3(relu, conv1x1, batch)), id, id, Linear1(Linear3(relu, conv1x1, layer)), id, id), Cell(id, Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, layer)), zero, Linear1(Linear3(hardswish, conv3x3, batch)))), Residual2(Cell(Linear1(Linear3(hardswish, conv3x3, layer)), Linear1(Linear3(relu, conv3x3, instance)), Linear1(Linear3(mish, conv1x1, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv3x3, layer)), id), Cell(Linear1(Linear3(relu, conv1x1, batch)), id, id, Linear1(Linear3(relu, conv3x3, batch)), id, id), Cell(id, Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, dconv3x3, layer)), zero, Linear1(Linear3(hardswish, dconv3x3, layer)))), Cell(Linear1(Linear3(relu, dconv3x3, instance)), zero, zero, id, zero, id)), Linear4(Residual2(Cell(Linear1(Linear3(hardswish, conv3x3, layer)), Linear1(Linear3(relu, conv3x3, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv3x3,



(a) D2 ::= `Linear3(D1, D1, D0)` | `Linear3(D0, D1, D1)` | `Linear4(D1, D1, D0, D0)`.

(b) D1 ::= `Linear3(C, C, D)` | `Linear4(C, C, C, D)` | `Residual3(C, C, D, D)`.

(c) D0 ::= `Linear3(C, C, CL)` | `Linear4(C, C, C, CL)` | `Residual3(C, C, CL, CL)`.

(d) D ::= `Linear2(CL, down)` | `Linear3(CL, CL, down)` | `Residual2(C, down, down)`.

(e) C ::= `Linear2(CL, CL)` | `Linear3(CL, CL)` | `Residual2(CL, CL, CL)`.

(f) OP ::= `zero` | `id` | BLOCK | `avg_pool`.

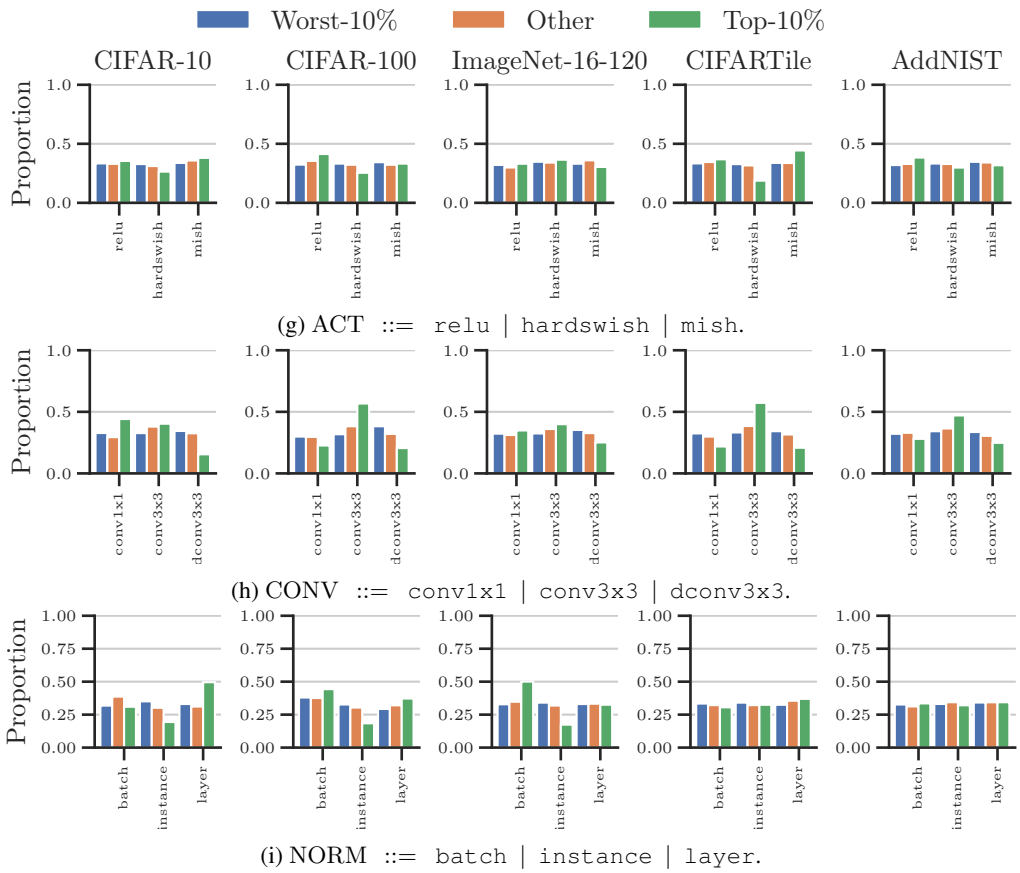
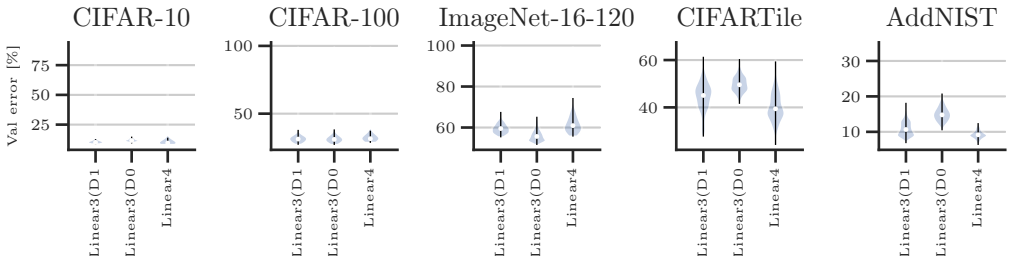
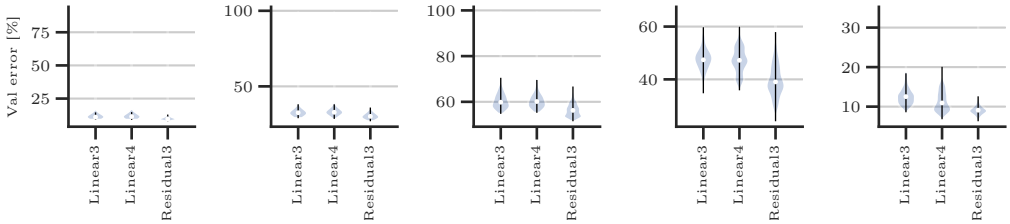


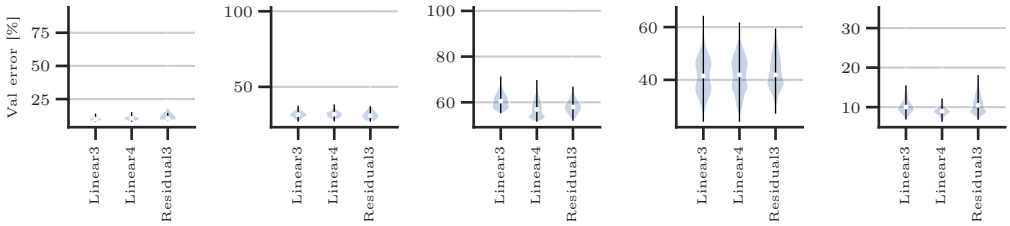
Figure 10: Comparison of the proportion of production rules in the worst-10% (blue), top-10% (green) and other (orange) neural architectures from our experiments in Section 6.



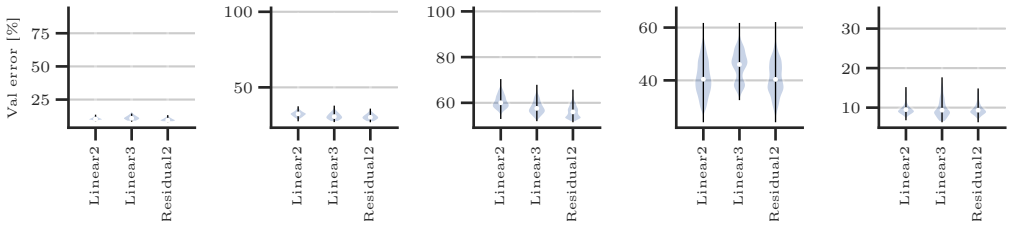
(a) D2 ::= `Linear3(D1, D1, D0)` | `Linear3(D0, D1, D1)` | `Linear4(D1, D1, D0, D0)`.



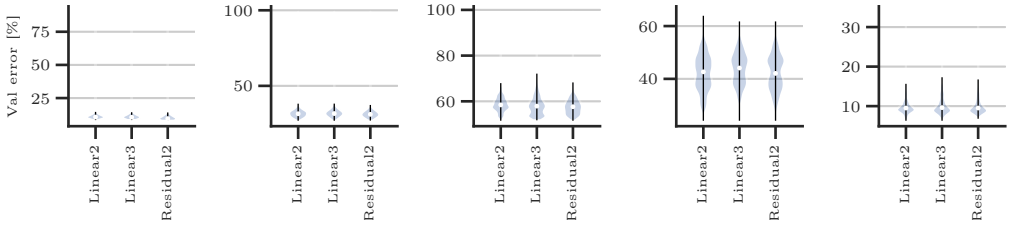
(b) D1 ::= `Linear3(C, C, D)` | `Linear4(C, C, C, D)` | `Residual3(C, C, D, D)`.



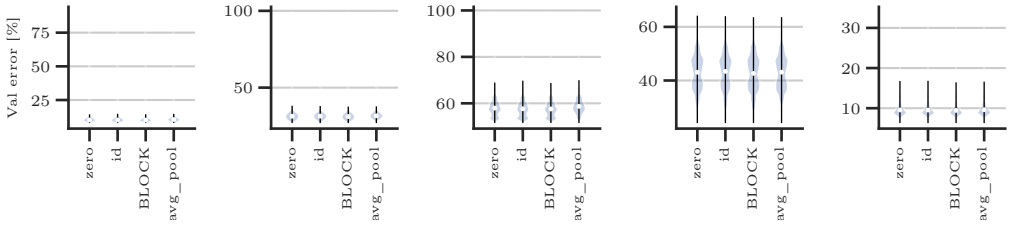
(c) D0 ::= `Linear3(C, C, CL)` | `Linear4(C, C, C, CL)` | `Residual3(C, C, CL, CL)`.



(d) D ::= `Linear2(CL, down)` | `Linear3(CL, CL, down)` | `Residual2(C, down, down)`.



(e) C ::= `Linear2(CL, CL)` | `Linear3(CL, CL)` | `Residual2(CL, CL, CL)`.



(f) OP ::= `zero` | `id` | BLOCK | `avg_pool`.

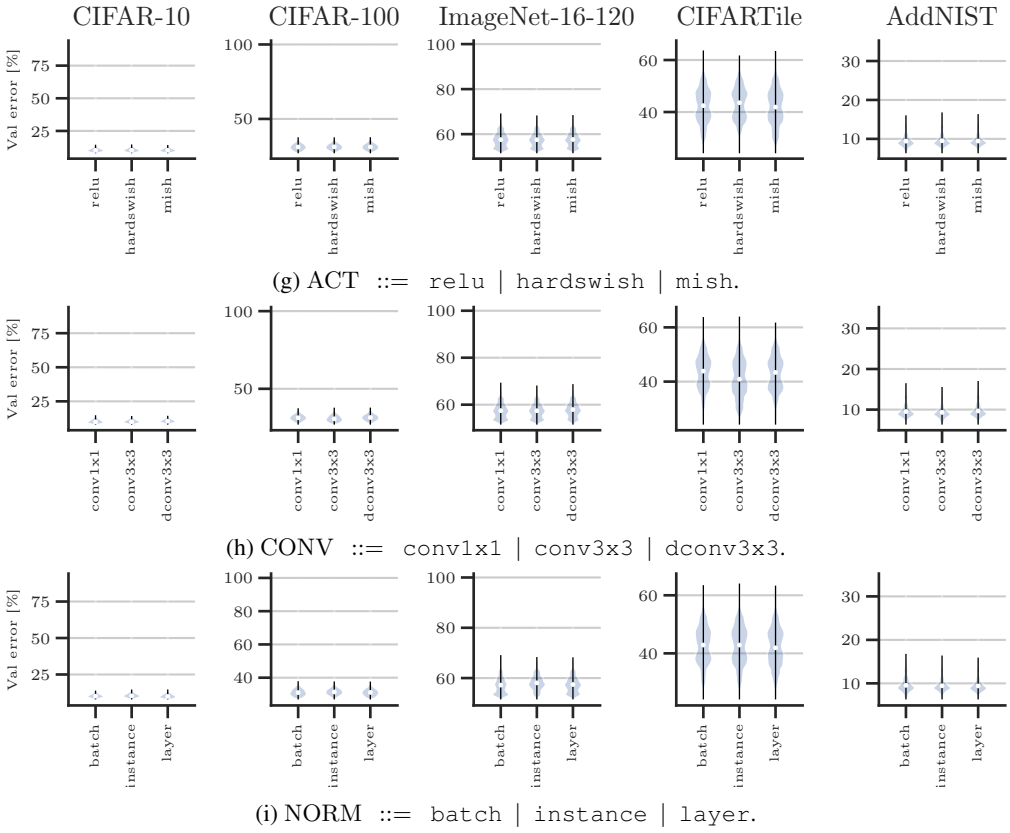


Figure 11: Marginalized performance of every production rule in our hierarchical NAS-Bench-201 search space from Section 6.

layer)), id), Cell(Linear1(Linear3(relu, conv1x1, batch)), id, id, Linear1(Linear3(relu, conv3x3, batch)), id, id), Cell(id, Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, layer)), zero, Linear1(Linear3(hardswish, conv3x3, batch)))), Residual2(Cell(Linear1(Linear3(hardswish, conv3x3, layer)), Linear1(Linear3(relu, conv3x3, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv3x3, layer)), id), Cell(Linear1(Linear3(relu, conv1x1, batch)), id, id, Linear1(Linear3(relu, conv3x3, batch)), id, id), Cell(id, Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, layer)), zero, Linear1(Linear3(hardswish, conv3x3, layer)))), Residual2(Cell(Linear1(Linear3(hardswish, conv3x3, layer)), Linear1(Linear3(relu, conv3x3, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv1x1, layer)), Linear1(Linear3(relu, conv3x3, layer)), id), Cell(Linear1(Linear3(relu, conv1x1, batch)), id, id, Linear1(Linear3(relu, conv3x3, batch)), id, id), Cell(id, Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, instance)), Linear1(Linear3(relu, conv1x1, layer)), zero, Linear1(Linear3(hardswish, conv3x3, layer)))), Cell(id, Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(mish, conv1x1, batch)), id, zero, id))) .

CIFAR-100 (mean test error 27.63 %, #params 0.962 MB, FLOPs 115.243 M):

Linear3(Residual3(Linear3(Cell(Linear3(mish, conv3x3, layer), avg_pool, Linear3(hardswish, conv1x1, instance), zero, Linear3(mish, conv3x3, batch), zero), Cell(Linear3(hardswish, dconv3x3, batch), zero, Linear3(hardswish, dconv3x3, batch), Linear3(relu, dconv3x3, batch), id, id), Cell(Linear3(mish, conv3x3, batch), zero, id, zero, Linear3(hardswish, dconv3x3, batch), id)), Linear2(Cell(id, zero, Linear3(mish, conv3x3, batch), zero, zero, Linear3(mish, conv1x1, batch)), Cell(zero, zero, zero, id, zero, avg_pool)), Cell(Linear3(relu, conv3x3, batch), zero, Linear3(hardswish, conv3x3, instance), id, id, avg_pool), Cell(id, id, zero, zero, id, id)), Residual3(Linear3(Cell(Linear3(mish, conv3x3, layer), id, Linear3(hardswish, dconv3x3, layer), Linear3(hardswish, dconv3x3, batch), Linear3(mish, conv3x3, instance), Linear3(mish, conv3x3, batch)), Cell(Linear3(hardswish, conv1x1, layer), id, Linear3(hardswish, dconv3x3, batch), Linear3(relu, conv3x3, layer), id, id), Cell(Linear3(relu, conv3x3, instance), zero, id, zero, Linear3(mish, conv3x3, batch), avg_pool)), Linear3(Cell(zero, id, Linear3(hardswish, conv1x1, layer), Linear3(mish, conv3x3, instance), Linear3(mish, conv3x3, instance), zero), Cell(Linear3(hardswish, conv1x1, layer), id, Linear3(hardswish, dconv3x3, batch), Linear3(relu, conv3x3, batch), id, id), Cell(Linear3(relu, conv3x3, instance), zero, id, zero, Linear3(mish, conv3x3, layer), avg_pool)), Residual2(Cell(zero, id, zero, Linear3(mish, conv3x3, layer), avg_pool, Linear3(mish, conv3x3, layer)), down, down), Residual2(Cell(zero, id, zero, Linear3(mish, conv3x3, batch), avg_pool, Linear3(mish, conv3x3, layer)), down, down)), Residual3(Linear3(Cell(Linear3(mish, conv3x3, layer), id, Linear3(hardswish, dconv3x3, layer), Linear3(hardswish, dconv3x3, batch), Linear3(mish, conv3x3, instance), Linear3(mish, conv3x3, batch)), Cell(Linear3(hardswish, conv1x1, layer), id, Linear3(hardswish, dconv3x3, batch), Linear3(relu, conv3x3, layer), id, id), Cell(Linear3(relu, conv3x3, instance), zero, id, zero, Linear3(mish, conv3x3, batch), avg_pool)), Linear3(Cell(Linear3(mish, conv3x3, batch), id, Linear3(hardswish, conv1x1, batch), Linear3(mish, conv3x3, instance), Linear3(mish, conv3x3, instance), zero), Cell(Linear3(hardswish, conv1x1, layer), id, Linear3(hardswish, dconv3x3, batch), Linear3(hardswish, dconv3x3, batch), id, id), Cell(Linear3(relu, conv3x3, instance), zero, id, zero, Linear3(mish, conv3x3, layer), avg_pool)), Residual2(Cell(zero, id, zero, Linear3(mish, conv3x3, layer), avg_pool, Linear3(mish, conv3x3, layer)), down, down), Residual2(Cell(zero, id, zero, Linear3(mish, conv3x3, batch), avg_pool, Linear3(mish, conv3x3, layer)), down, down)))

ImageNet-16-120 (mean test error 52.78 %, #params 0.626 MB, FLOPs 23.771 M):

Linear3(Linear4(Residual2(Cell(id, avg_pool, id, id, Linear3(relu, dconv3x3, layer), zero), Cell(Linear3(hardswish, conv1x1, batch), zero, zero, Linear3(mish, dconv3x3, layer), zero, zero), Cell(Linear3(relu, dconv3x3, layer), Linear3(mish, dconv3x3, layer), zero, Linear3(hardswish, conv3x3, layer), Linear3(relu, dconv3x3, instance), Linear3(hardswish, conv3x3, instance))), Linear2(Cell(zero, Linear3(relu, conv3x3, layer), Linear3(mish, conv1x1, batch), Linear3(mish, conv1x1, batch), avg_pool, Linear3(relu, conv3x3, layer)), Cell(id, id, Linear3(mish, conv3x3, layer), Linear3(relu, conv3x3, instance), id, id)), Residual2(Cell(zero, avg_pool, Linear3(mish, conv1x1, batch), Linear3(mish, conv1x1, layer), zero, zero), Cell(id, Linear3(relu, dconv3x3, layer), zero,

zero, Linear3(relu, dconv3x3, instance), zero), Cell(id, Linear3(relu, conv3x3, layer), id, zero, zero, id)), Cell(zero, Linear3(hardswish, conv3x3, layer), avg_pool, zero, Linear3(hardswish, conv1x1, layer), id)), Residual3(Residual2(Cell(Linear3(relu, conv1x1, instance), Linear3(mish, conv1x1, layer), Linear3(mish, conv1x1, instance), zero, Linear3(hardswish, dconv3x3, layer), id), Cell(id, avg_pool, avg_pool, Linear3(relu, conv1x1, instance), id, zero), Cell(avg_pool, Linear3(mish, conv3x3, instance), Linear3(mish, conv1x1, instance), Linear3(relu, dconv3x3, batch), id, Linear3(hardswish, conv3x3, instance))), Linear2(Cell(zero, Linear3(relu, conv3x3, layer), Linear3(mish, conv1x1, batch), Linear3(mish, conv1x1, batch), avg_pool, Linear3(relu, conv3x3, instance)), Cell(id, zero, Linear3(mish, conv3x3, layer), Linear3(relu, conv3x3, instance), id, id)), Residual2(Cell(Linear3(mish, conv3x3, layer), Linear3(mish, conv1x1, batch), id, Linear3(mish, conv1x1, layer), zero, id), down, down), Residual2(Cell(Linear3(relu, conv3x3, layer), zero, Linear3(relu, dconv3x3, layer), Linear3(mish, conv1x1, layer), zero, id), down, down)), Residual3(Residual2(Cell(Linear3(mish, conv1x1, instance), Linear3(mish, conv1x1, layer), Linear3(mish, conv1x1, instance), avg_pool, Linear3(hardswish, dconv3x3, layer), id), Cell(id, avg_pool, avg_pool, Linear3(relu, conv1x1, instance), id, zero), Cell(avg_pool, Linear3(mish, conv3x3, instance), Linear3(mish, conv1x1, instance), Linear3(relu, dconv3x3, batch), id, Linear3(hardswish, conv3x3, instance))), Linear2(Cell(zero, Linear3(relu, conv3x3, layer), Linear3(mish, conv1x1, batch), Linear3(mish, conv1x1, batch), avg_pool, Linear3(relu, conv3x3, layer)), Cell(id, zero, Linear3(mish, conv3x3, layer), Linear3(relu, conv3x3, instance), id, id)), Residual2(Cell(Linear3(relu, conv3x3, layer), avg_pool, id, Linear3(mish, conv3x3, instance), zero, id), down, down), Residual2(Cell(Linear3(relu, conv3x3, layer), zero, Linear3(relu, dconv3x3, instance), Linear3(mish, conv1x1, layer), zero, id), down, down)))

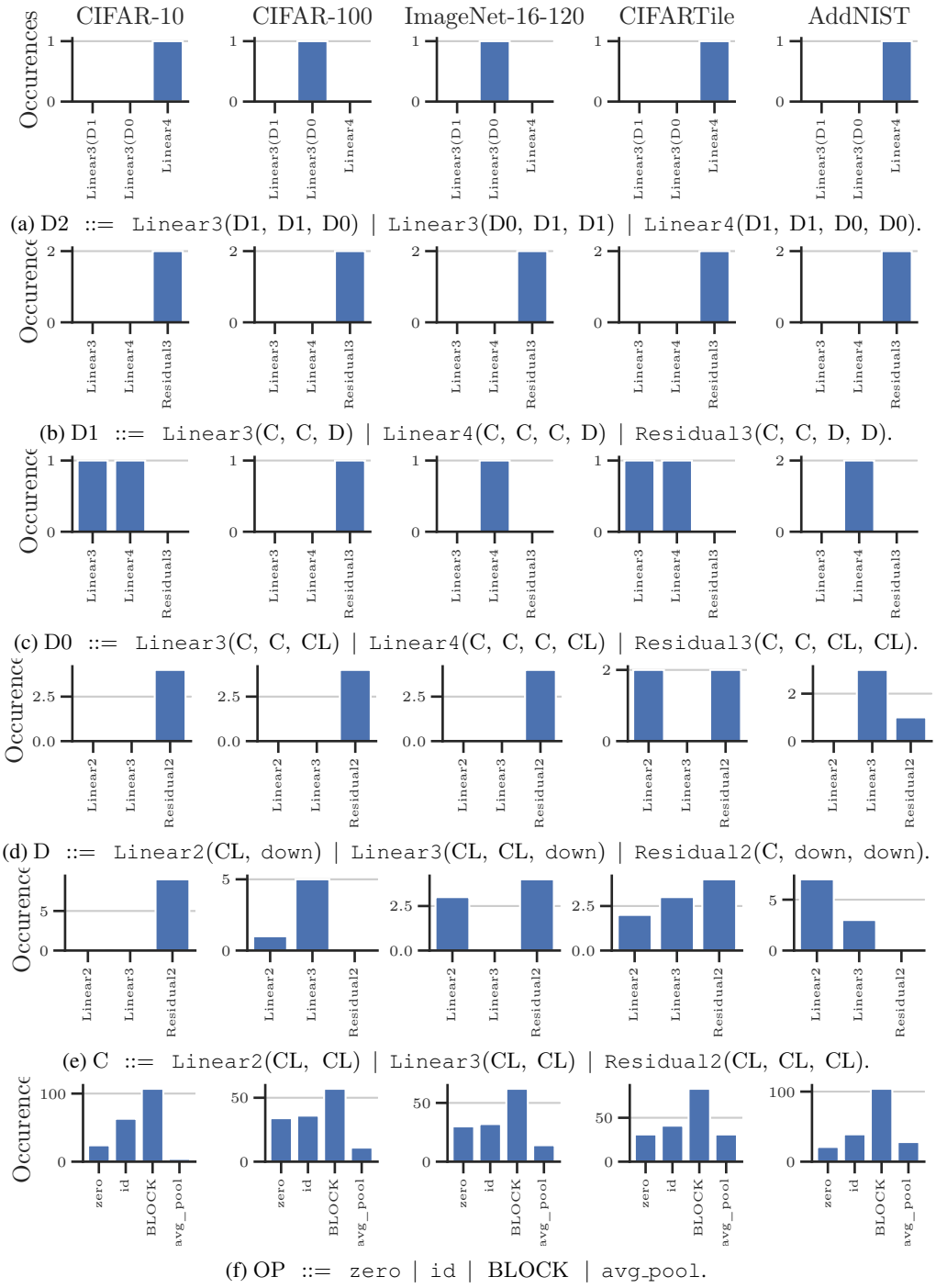
CIFARTile (mean test error $30.33\,\%$, #params $2.356\,\mathrm{MB}$, FLOPs $372.114\,\mathrm{M}$):

Linear4(Residual3(Residual2(Cell(Linear3(hardswish, conv3x3, instance), id, zero, Linear3(relu, dconv3x3, instance), Linear3(mish, conv1x1, instance), avg_pool), Cell(avg_pool, avg_pool, id, zero, Linear3(hardswish, conv3x3, batch), avg_pool), Cell(Linear3(relu, dconv3x3, instance), zero, id, Linear3(relu, dconv3x3, layer), id, id)), Residual2(Cell(zero, zero, Linear3(mish, conv1x1, instance), Linear3(mish, conv3x3, batch), zero, id), Cell(Linear3(mish, conv3x3, instance), zero, Linear3(relu, dconv3x3, batch), id, Linear3(mish, conv3x3, batch), id), Cell(Linear3(hardswish, dconv3x3, batch), Linear3(relu, conv3x3, batch), Linear3(relu, conv1x1, batch), zero, Linear3(relu, conv3x3, batch), id)), Linear2(Cell(Linear3(relu, dconv3x3, layer), Linear3(mish, conv1x1, layer), id, zero, Linear3(mish, conv3x3, batch), Linear3(relu, dconv3x3, layer)), down), Linear2(Cell(id, Linear3(hardswish, conv1x1, layer), id, Linear3(relu, conv1x1, instance), avg_pool, Linear3(relu, conv1x1, layer)), down)), Residual3(Residual2(Cell(id, avg_pool, avg_pool, Linear3(hardswish, dconv3x3, instance), Linear3(mish, conv1x1, layer), Linear3(hardswish, dconv3x3, instance)), Cell(id, id, Linear3(relu, dconv3x3, layer), id, id, zero), Cell(Linear3(relu, conv3x3, layer), id, avg_pool, Linear3(mish, dconv3x3, instance), Linear3(relu, conv1x1, layer), zero)), Residual2(Cell(Linear3(mish, conv3x3, batch), Linear3(mish, conv3x3, instance), zero, avg_pool, avg_pool, Linear3(mish, conv1x1, batch)), Cell(Linear3(mish, conv1x1, batch), Linear3(relu, dconv3x3, layer), zero, id, avg_pool, avg_pool), Cell(avg_pool, Linear3(hardswish, conv1x1, instance), id, avg_pool, avg_pool, Linear3(hardswish, conv1x1, instance))), Residual2(Cell(Linear3(relu, dconv3x3, batch), avg_pool, id, avg_pool, id, zero), down, down), Residual2(Cell(zero, zero, Linear3(relu, dconv3x3, batch), avg_pool, Linear3(hardswish, conv1x1, instance), avg_pool), down, down)), Linear4(Linear3(Cell(Linear3(hardswish, conv3x3, batch), Linear3(hardswish, conv3x3, batch), Linear3(relu, conv1x1, instance), id, Linear3(relu, conv1x1, layer), Linear3(relu, conv3x3, layer)), Cell(id, Linear3(relu, conv3x3, instance), Linear3(hardswish, conv1x1, instance), Linear3(relu, conv3x3, layer), avg_pool, Linear3(mish, conv1x1, layer)), Cell(zero, zero, id, Linear3(relu, conv3x3, batch), id, Linear3(relu, conv1x1, layer))), Linear3(Cell(Linear3(hardswish, conv3x3, batch), Linear3(hardswish, conv3x3, batch), Linear3(relu, conv1x1, instance), Linear3(relu, dconv3x3, layer), Linear3(mish, conv1x1, layer), Linear3(relu, conv3x3, batch)), Cell(id, Linear3(relu, conv3x3, instance), Linear3(hardswish, conv1x1, instance), Linear3(relu, dconv3x3, instance), avg_pool, Linear3(mish, conv1x1, layer)), Cell(zero, zero, id, Linear3(relu, conv3x3, batch), id, avg_pool)), Linear3(Cell(id, id, avg_pool, Linear3(mish, conv1x1, layer), Linear3(mish, conv3x3, batch), zero), Cell(id, Linear3(relu, conv1x1, batch), avg_pool, Linear3(relu, conv1x1, layer), avg_pool, zero), Cell(zero, Linear3(relu, conv1x1, batch), Linear3(mish, dconv3x3, batch), Linear3(mish, conv1x1, batch), id, id)), Cell(id, Linear3(hardswish, conv1x1, layer), zero, id, zero, id)), Linear3(Linear2(Cell(id, zero, Linear3(mish, dconv3x3, instance), Linear3(mish, conv3x3, batch), Linear3(mish,

dconv3x3, instance), Linear3(relu, conv1x1, instance)), Cell(Linear3(relu, dconv3x3, instance), avg_pool, Linear3(mish, conv1x1, instance), Linear3(hardswish, dconv3x3, instance), id, Linear3(hardswish, conv1x1, layer))), Linear2(Cell(zero, zero, Linear3(mish, dconv3x3, instance), Linear3(relu, conv3x3, instance), Linear3(hardswish, conv3x3, batch), avg_pool), Cell(id, id, Linear3(hardswish, conv1x1, instance), avg_pool, zero, Linear3(hardswish, conv3x3, batch))), Cell(avg_pool, Linear3(mish, dconv3x3, layer), zero, avg_pool, avg_pool, zero))) .

AddNIST (test error $6.33\,\%$, #params $2.853\,\mathrm{MB}$, FLOPs $593.856\,\mathrm{M}$):

Linear4(Residual3(Linear3(Cell(id, Linear3(hardswish, dconv3x3, batch), Linear3(relu, conv1x1, layer), Linear3(mish, conv3x3, batch), avg_pool, zero), Cell(zero, zero, avg_pool, id, avg_pool, Linear3(hardswish, conv1x1, instance)), Cell(Linear3(relu, conv3x3, layer), id, zero, Linear3(mish, conv3x3, instance), id, avg_pool)), Linear2(Cell(id, Linear3(relu, conv3x3, layer), Linear3(relu, conv3x3, layer), Linear3(hardswish, conv3x3, batch), id, Linear3(relu, conv3x3, layer)), Cell(Linear3(mish, conv3x3, instance), id, Linear3(mish, conv3x3, batch), id, avg_pool, id)), Linear3(Cell(zero, id, Linear3(relu, dconv3x3, instance), Linear3(relu, dconv3x3, layer), Linear3(relu, dconv3x3, instance), Linear3(mish, conv3x3, batch)), Cell(Linear3(mish, conv1x1, instance), zero, Linear3(relu, conv3x3, instance), id, zero, Linear3(relu, conv3x3, batch)), down), Linear3(Cell(zero, avg_pool, Linear3(hardswish, dconv3x3, layer), Linear3(relu, conv3x3, layer), Linear3(hardswish, conv1x1, instance), Linear3(hardswish, conv3x3, batch)), Cell(Linear3(hardswish, conv3x3, batch), Linear3(hardswish, conv1x1, layer), Linear3(mish, conv1x1, batch), id, Linear3(hardswish, conv3x3, batch), zero), down)), Residual3(Linear2(Cell(Linear3(mish, conv1x1, layer), avg_pool, Linear3(hardswish, dconv3x3, batch), Linear3(mish, dconv3x3, batch), id, Linear3(mish, conv3x3, layer)), Cell(zero, Linear3(relu, dconv3x3, layer), Linear3(hardswish, conv3x3, instance), avg_pool, avg_pool, zero)), Linear3(Cell(Linear3(relu, conv3x3, batch), id, Linear3(relu, conv3x3, layer), Linear3(mish, conv1x1, instance), id, Linear3(relu, dconv3x3, batch)), Cell(Linear3(mish, conv3x3, batch), Linear3(mish, conv1x1, instance), Linear3(mish, conv3x3, instance), zero, Linear3(mish, dconv3x3, layer), Linear3(relu, conv3x3, batch)), Cell(avg_pool, Linear3(mish, conv1x1, instance), Linear3(relu, conv3x3, batch), avg_pool, id, Linear3(mish, dconv3x3, batch))), Linear3(Cell(zero, avg_pool, Linear3(hardswish, dconv3x3, layer), Linear3(relu, conv3x3, batch), Linear3(hardswish, conv1x1, batch), Linear3(hardswish, conv3x3, batch)), Cell(avg_pool, Linear3(hardswish, dconv3x3, layer), Linear3(mish, conv1x1, batch), id, Linear3(hardswish, conv3x3, batch), zero), down), Residual2(Cell(zero, Linear3(mish, conv1x1, instance), Linear3(hardswish, conv1x1, instance), avg_pool, Linear3(relu, conv1x1, layer), Linear3(hardswish, dconv3x3, batch)), down, down)), Linear4(Linear2(Cell(Linear3(relu, conv3x3, instance), id, Linear3(relu, conv3x3, batch), avg_pool, zero, id), Cell(avg_pool, Linear3(hardswish, conv3x3, layer), avg_pool, Linear3(mish, conv3x3, batch), Linear3(relu, conv3x3, batch), id)), Linear2(Cell(Linear3(mish, conv1x1, layer), avg_pool, Linear3(hardswish, dconv3x3, batch), Linear3(mish, dconv3x3, batch), id, Linear3(mish, conv3x3, layer)), Cell(zero, Linear3(relu, dconv3x3, layer), Linear3(hardswish, conv3x3, instance), avg_pool, avg_pool, zero)), Linear2(Cell(id, Linear3(relu, conv3x3, instance), Linear3(relu, conv3x3, layer), Linear3(hardswish, dconv3x3, batch), id, Linear3(relu, conv3x3, layer)), Cell(Linear3(mish, conv1x1, batch), id, avg_pool, id, avg_pool, id)), Cell(id, Linear3(relu, conv3x3, layer), Linear3(mish, conv1x1, instance), Linear3(hardswish, conv3x3, batch), Linear3(mish, dconv3x3, instance), Linear3(hardswish, conv1x1, instance))), Linear4(Linear2(Cell(Linear3(relu, conv3x3, instance), id, Linear3(relu, conv3x3, batch), avg_pool, zero, id), Cell(zero, Linear3(relu, conv3x3, batch), avg_pool, Linear3(mish, conv3x3, batch), Linear3(relu, dconv3x3, instance), id)), Linear3(Cell(Linear3(relu, conv3x3, batch), id, Linear3(relu, conv3x3, layer), Linear3(mish, conv1x1, layer), id, Linear3(relu, dconv3x3, instance)), Cell(Linear3(mish, conv3x3, batch), Linear3(mish, conv1x1, instance), Linear3(hardswish, dconv3x3, instance), zero, Linear3(mish, dconv3x3, layer), Linear3(relu, conv3x3, batch)), Cell(avg_pool, Linear3(mish, conv1x1, instance), Linear3(relu, conv3x3, batch), avg_pool, id, Linear3(mish, dconv3x3, batch))), Linear2(Cell(id, Linear3(relu, conv3x3, layer), Linear3(hardswish, conv3x3, layer), Linear3(hardswish, dconv3x3, batch), id, Linear3(relu, conv3x3, layer)), Cell(Linear3(mish, conv3x3, batch), id, avg_pool, id, avg_pool, id)), Cell(id, Linear3(relu, conv3x3, layer), Linear3(mish, conv1x1, instance), Linear3(hardswish, conv3x3, batch), Linear3(mish, dconv3x3, instance), Linear3(mish, conv3x3, instance)))) .



(a) D2 ::= `Linear3(D1, D1, D0)` | `Linear3(D0, D1, D1)` | `Linear4(D1, D1, D0, D0)`.

(b) D1 ::= `Linear3(C, C, D)` | `Linear4(C, C, C, D)` | `Residual3(C, C, D, D)`.

(c) D0 ::= `Linear3(C, C, CL)` | `Linear4(C, C, C, CL)` | `Residual3(C, C, CL, CL)`.

(d) D ::= `Linear2(CL, down)` | `Linear3(CL, CL, down)` | `Residual2(C, down, down)`.

(e) C ::= `Linear2(CL, CL)` | `Linear3(CL, CL)` | `Residual2(CL, CL, CL)`.

(f) OP ::= `zero` | `id` | BLOCK | `avg_pool`.

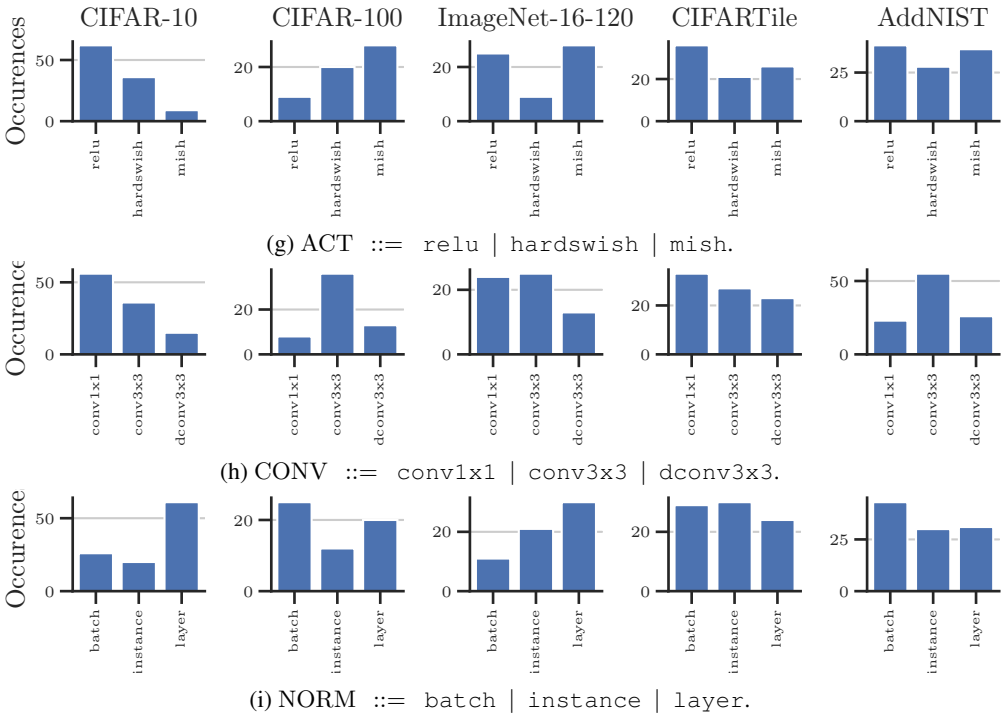


Figure 12: Summary of the distribution of topological operators and primitive operations of the best architectures on the hierarchical NAS-Bench-201 search space.

H BEST PRACTICES CHECKLIST FOR NAS RESEARCH

NAS research has faced challenges with reproducibility and fair empirical comparisons for a long time (Li & Talwalkar, 2020; Yang et al., 2020a). In order to promote fair and reproducible NAS research, Lindauer & Hutter (2020) created a best practices checklist for NAS research. Below, we address all points on the checklist.

1. **Best Practices for Releasing Code**
   (a) *Did you release code for the training pipeline used to evaluate the final architectures?, Did you release code for the search space?, Did you release code for your NAS method?* [Yes] All code can be found at `https://anonymous.4open.science/r/iclr23_tdnafs`.
   (b) *Did you release the hyperparameters used for the final evaluation pipeline, as well as random seeds?* [Yes] We provide experimental details (including hyperparameters as well as random seeds) in Section 6 and Appendix G.2.
   (c) *Did you release hyperparameters for your NAS method, as well as random seeds?* [Yes] We discuss implementation details (including hyperparameters as well as random seeds) of our NAS method in Section 6 and Appendix G.1.
2. **Best practices for comparing NAS methods**
   (a) *For all NAS methods you compare, did you use exactly the same NAS benchmark, including the same dataset (with the same training-test split), search space and code for training the architectures and hyperparameters for that code?* [Yes] We always used the same training pipelines during search and final evaluation.
   (b) *Did you control for confounding factors (different hardware, versions of deep learning libraries, different runtimes for the different methods)?* [Yes] We kept hardware, software versions, and runtimes fixed across our experiments to reduce effects of confounding factors.

(c) *Did you run ablation studies?* [Yes] We compared different kernels (hWL vs. WL) and investigated the surrogate performance in Section 6. We also analyzed the distribution of architectures and frequency of production rules in Appendix G.3.

(d) *Did you use the same evaluation protocol for the methods being compared?* [Yes]

(e) *Did you compare performance over time?* [Yes] We plotted results over the number of iterations, as typically done for black-box optimizers, and report the total search cost in Appendix G.3.

(f) *Did you compare to random search?* [Yes]

(g) *Did you perform multiple runs of your experiments and report seeds?* [Yes] We ran all computationally intensive experiments over three seeds, and computationally less-demanding experiments over 20 seeds.

(h) *Did you use tabular or surrogate benchmarks for in-depth evaluations?* [N/A] At the time of this work, there existed no surrogate benchmark for hierarchical NAS.

3. **Best practices for reporting important details**

(a) *Did you report how you tuned hyperparameters, and what time and resources this required?* [N/A] We have not tuned any hyperparameter.

(b) *Did you report the time for the entire end-to-end NAS method (rather than, e.g., only for the search phase?* [Yes] We report search times in Appendix G.3. Since the training protocols are exactly the same for the search and final evaluation (except for CIFAR-10), there are no additional costs for final evaluation.

(c) *Did you report all the details of your experimental setup?* [Yes] We report all experimental details in Section 6 and Appendix G.2.