Towards Discovering Neural Architectures from Scratch

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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 [1], 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., [2–4]), success in automatically finding truly novel architectural patterns has been very scarce [5, 6]. 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 [7–9].

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, taking a large step towards discovering neural architectures from scratch. 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

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

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.

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

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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 and propose to design these spaces with CFGs (Sec. 2).
- We propose BANAT, a Bayesian Optimization (BO) strategy that uses a tailored kernel to efficiently and effectively search over our huge search spaces (Sec. 3).
- We find 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 (Sec. 5).

We open source our algebraic NAS approach. For discussion and limitations see App. A.

2 Algebraic neural architecture search

In this section, we develop an algebraic view on Neural Architecture Search (NAS).

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 $n \geq 0$ [10]. 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 as shown in Eq. 1. 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: $\omega' = \texttt{Linear}(x_1,\ x_1,\ \texttt{fc}), x_1 = \texttt{Residual}(\texttt{conv},\ \texttt{id},\ \texttt{conv})$.

Algebraic NAS Consequently, we formulate our algebraic view on NAS, where we search over algebraic architecture terms $\omega \in \Omega$ representing their associated architectures $\Phi(\omega)$: $\arg\min_{\omega\in\Omega} f(\Phi(\omega))$,where $f(\cdot)$ is an error measure that we seek to minimize, e.g., validation error. Thus, our search problem is to discover algebraic architecture terms ω, which can be part of very expressive search spaces Ω. Even though the ideas above are very powerful, two questions immediately come to mind: (1) How to construct architecture term spaces Ω? (subsequent paragraph), and (2) How to optimize over these huge spaces? (subsequent section).

Constructing neural architecture terms with context-free grammars To construct algebraic architecture terms, we utilize *Context-Free Grammars (CFGs)* [11] 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 $P = \{A \to \beta | A \in N, \beta \in (N \cup \Sigma)^*\}$, where the asterisk $*$ denotes the Kleene star operation [12], and a start symbol $S \in N$. For example, consider the following CFG in extended Backus-Naur form [13] (see App. D for a detailed description): S ::= `Linear`(S, S, S) | `Residual`(S, S, S) | `conv` | `id` | `fc` Fig. 1 depicts the derivation of the algebraic architecture term from Eq. 1 and makes the connection to the associated 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. We can construct very expressive search spaces (e.g., see App. K.1) as well as unify popular search spaces from the literature with our search space design (App. H). However, there is of course no single search space that can construct any neural architecture.

In App. E we further augment the capabilities of CFGs so that we can incorporate constraints, foster regularity, and handle changes in the spatial resolution (and number of channels).

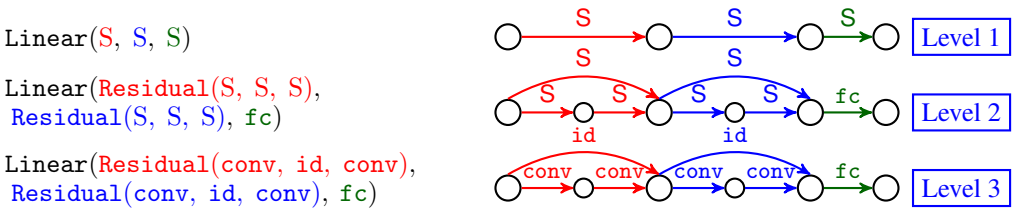

Figure 1: Derivations of algebraic terms (left) correspond to edge replacements [14–16] in the associated neural architecture (right). See App. C for the topological operators and primitive computations.

3 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. Our search strategy, BANAT combines a Gaussian Process (GP) with a tailored kernel that leverages the hierarchical structure of algebraic neural architecture terms (see below). For a more detailed explanation of the BO mechanism and our parallelization strategy, please refer to App. I.

Inspired by the state-of-the-art BO approach for NAS [17], we adopt the WL graph kernel [18] 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. Note that 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 Fig. 1), Thus, we propose a novel hierarchical kernel design which assigns a WL kernel to each hierarchy and combines them.To this end, we introduce fold operators F_l, that removes algebraic terms beyond the l-th hierarchical level. E.g., for the algebraic term ω in Eq. 1.

$$F_3(\omega) = \omega = \texttt{Linear}(\texttt{Residual}(\texttt{conv, id, conv}), \texttt{Residual}(\texttt{conv, id, conv}), \texttt{fc}), \quad (2)$$
$$F_2(\omega) = \texttt{Linear}(\texttt{Residual, Residual, fc}) \quad , \quad F_1(\omega) = \texttt{Linear} \quad .$$

Note the similarity to the derivations in Fig. 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:

$$k_{hWL}(\omega_i, \omega_j) = \sum_{l=2}^{L} \lambda_l \cdot k_{WL}(\Phi(F_l(\omega_i)), \Phi(F_l(\omega_j))) \quad , \quad (3)$$

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 hierarchical 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 Sec. 5.

4 Related work

Previous approaches, e.g., used reinforcement learning [19, 20], evolution [21], gradient descent [22], or Bayesian Optimization (BO) [17, 23, 24]. To enable the effective use of BO on graph-like inputs for NAS, previous works have proposed to use a GP with specialized kernels [17, 23], encoding schemes [24, 25], or graph neural networks as surrogate model [26–28]. Different to prior works, we explicitly leverage the hierarchical construction of architectures for modeling. Most previous works focused on finding a shared cell [29] with a fixed macro architecture while only few works

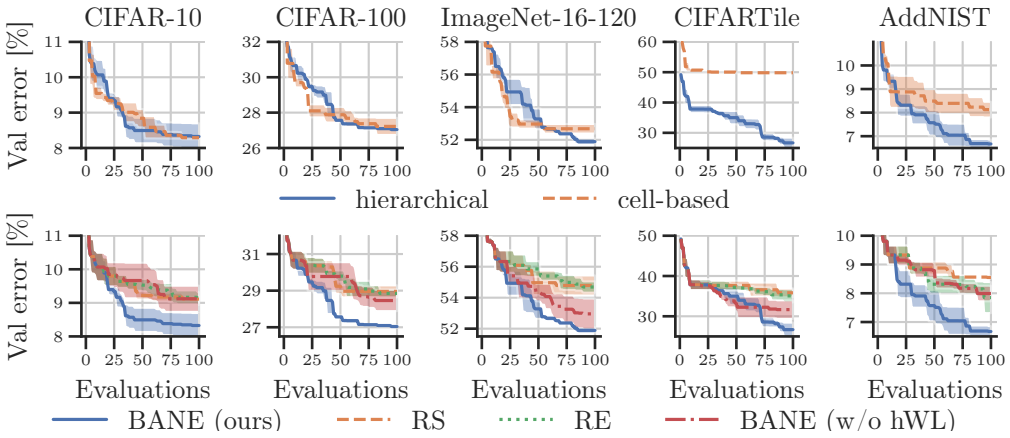

Figure 2: We compare cell-based vs. hierarchical search space using BANAT (top) and compare it to common baselines (bottom). We plot mean and ± 1 standard error.

considered more expressive hierarchical [4, 9, 30–35] or grammar-based [36–53] approaches. Similar to the former, 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. Different to the latter grammar-based works we construct entire architectures with spatial resolution changes across multiple branches, and propose techniques to incorporate constraints and foster regularity. Please refer to App. J for an extended discussion of related work.

5 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?; and **Q3** Does leveraging the hierarchical information improve performance? To answer these questions, we introduce a hierarchical search space (App. K.1) based on the popular NAS-Bench-201 search space [54] and experimentally answer them in the affirmative. For evaluation details, please refer to App. K.4. We also provide the further details and results in App. K.

Fig. 2 (top) 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 (App. K.5); this is superior to the state-of-the-art method Shapley-NAS (i.e., $53.15\,\%$) [55] and on par with the *optimal* architecture of the cell-based NAS-Bench-201 search space (i.e., $52.69\,\%$ with $0.866\,\mathrm{MB}$). Fig. 2 (bottom) shows that BANAT is superior to common baselines (answering **Q2**) and that leveraging hierarchical information clearly improves performance (answering **Q3**). The analysis in Fig. 11 shows that incorporating hierarchical information improves modeling, especially on smaller amounts of training data; this provides further evidence for answering **Q3**.

6 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. Our experiments indicate that both our search space design and algorithm can yield strong performance over existing baselines.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] Our abstract and introduction accurately reflect our paper's contribution.
   (b) Did you describe the limitations of your work? [Yes] See Sec. A.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See App. B.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes] We discuss the ethics guidelines in App. B.
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [N/A] We did not include theoretical results.
   (b) Did you include complete proofs of all theoretical results? [N/A] We did not include theoretical results.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] `https://anonymous.4open.science/status/neurips22_workshop-tdnafs`.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] We report all training details in App. K.

(c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We plotted ± 1 standard error for our experiments in Sec. 5 over 3 or 20 trials for the search or surrogate experiments, respectively.

(d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] We report compute time and type of resource in App. K.

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(a) If your work uses existing assets, did you cite the creators? [Yes] We cite the creators of all datasets and search strategies used.

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(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A] We did not run experiments with human subjects.

A 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 architectures with a single search space based on our grammar-based approach from Sec. 2, our search spaces still significantly increase the expressiveness, including the ability to represent common search spaces from the literature (see App. H for how we can represent the search spaces of DARTS, Auto-Deeplab, the hierarchical cell search space of Liu et al. [30], 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 (Sec. 5). 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).

B Broader impact

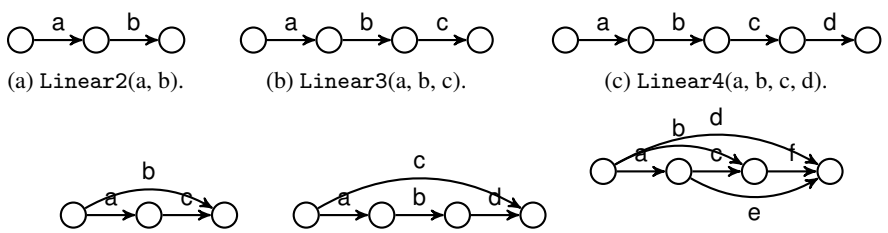
NAS has immense potential to facilitate systematic, automated discovery of high-performing (novel) architecture designs. However, the restrictive cell-based search spaces most commonly used in NAS render it impossible to discover truly novel neural architectures. With our general formalism based on algebraic 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.

C From terminals to primitive computations and topological operators

Table 1 and Fig. 3 describe the primitive computations and topological operators used throughout our experiments in Sec. 5 and App. K, 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`	$\texttt{conv3x3}_{s=1}\texttt{(conv3x3}_{s=2}\texttt{(x)) + Conv}_{k=1,s=1}\texttt{(AvgPool}_{k=2,s=2}\texttt{(x))}$
`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 3: 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.

D Extended Backus-Naur form

The (extended) Backus-Naur form [13] 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., $\mathrm{S} ::= \texttt{Residual}(\mathrm{S},\ \mathrm{S},\ \texttt{id})$. 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., $\mathrm{S} ::= \texttt{Linear}(\mathrm{S},\ \mathrm{S},\ \mathrm{S}) \mid \texttt{Residual}(\mathrm{S},\ \mathrm{S},\ \texttt{id}) \mid \texttt{conv}$.

E Augmenting the capabilities of context-free grammars

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 App. G.

Fostering regularity through substitution To implement intermediate variables x_i as described in Sec. 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 [54], while also being able to represent more expressive search spaces (e.g., see App. K.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 [29] or only allowed for linear macro architectures [4]. While this produced impressive performance on popular benchmarks [2–4], 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.

F 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

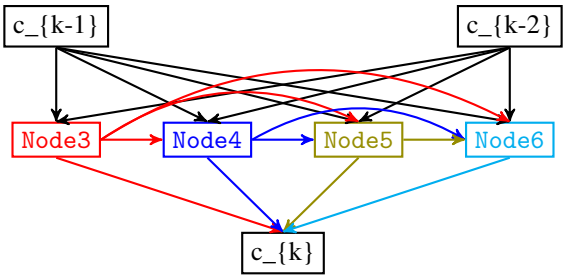


Figure 4: Visualization of the `Darts` topological operator.

can then recursively compute the size of the search space as follows:

$$f(\mathrm{A}) = \sum_{p \in P_{\mathrm{A}}} \begin{cases} 1 & , \mu(p) = \emptyset, \\ \prod_{\mathrm{A}' \in \mu(p)} f(\mathrm{A}') & , otherwise \end{cases} . \tag{4}$$

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.

G 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 Sec. 2 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.

H Common search spaces from the literature

In App. K.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 [22], Auto-DeepLab search space [4], hierarchical cell search space [30], Mobile-net search space [32], and hierarchical random graph generator search space [9]. For implementation details we refer to the respective works.

DARTS search space

The DARTS search space [22] consists of a fixed macro architecture and a cell, i.e., a seven node directed acyclic graph (`Darts`; see Fig. 4 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 (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:

$$
\begin{aligned}
\text{DARTS} &::= \texttt{Darts}(\text{NODE3},\ \text{NODE4},\ \text{NODE5},\ \text{NODE6}) \\
\text{NODE3} &::= \texttt{Node3}(\text{OP},\ \text{OP}) \\
\text{NODE4} &::= \texttt{Node4}(\text{OP},\ \text{OP},\ \text{OP}) \\
\text{NODE5} &::= \texttt{Node5}(\text{OP},\ \text{OP},\ \text{OP},\ \text{OP}) \\
\text{NODE6} &::= \texttt{Node6}(\text{OP},\ \text{OP},\ \text{OP},\ \text{OP},\ \text{OP}) \\
\text{OP} &::= \texttt{sep_conv_3x3} \mid \texttt{sep_conv_5x5} \mid \texttt{dil_conv_3x3} \mid \texttt{dil_conv_5x5} \\
&\quad \mid \texttt{max_pool} \mid \texttt{avg_pool} \mid \texttt{id} \mid \texttt{zero} \quad ,
\end{aligned}
\tag{5}
$$

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 [4] 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. [22] and, thus, we can re-use the CFG from Eq. 5. 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 Sec. 2 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:

$$
\begin{aligned}
\text{D4} &::= \texttt{Same}(\texttt{CELL},\ \text{D4}) \mid \texttt{Down}(\texttt{CELL},\ D8) \\
\text{D8} &::= \texttt{Up}(\texttt{CELL},\ \text{D4}) \mid \texttt{Same}(\texttt{CELL},\ \text{D8}) \mid \texttt{Down}(\texttt{CELL},\ \text{D16}) \\
\text{D16} &::= \texttt{Up}(\texttt{CELL},\ \text{D8}) \mid \texttt{Same}(\texttt{CELL},\ \text{D16}) \mid \texttt{Down}(\texttt{CELL},\ \text{D32}) \\
\text{D32} &::= \texttt{Up}(\texttt{CELL},\ \text{D16}) \mid \texttt{Same}(\texttt{CELL},\ \text{D32}) \quad ,
\end{aligned}
\tag{6}
$$

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 Eq. 5.

Hierarchical cell search space

The hierarchical cell search space [30] 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

$$
\begin{aligned}
\text{LEVEL3} &::= \texttt{DAG5}(\underbrace{\text{LEVEL2},\ \ldots,\ \text{LEVEL2}}_{\times 10}) \\
\text{LEVEL2} &::= \texttt{M1} \mid \texttt{M2} \mid \texttt{M3} \mid \texttt{M4} \mid \texttt{M5} \mid \texttt{M6} \mid \texttt{zero} \quad ,
\end{aligned}
\tag{7}
$$

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

$$
\begin{aligned}
\text{LEVEL2} &::= \texttt{DAG4}(\underbrace{\text{LEVEL1},\ \ldots,\ \text{LEVEL1}}_{\times 6}) \\
\text{LEVEL1} &::= \texttt{id} \mid \texttt{max_pool} \mid \texttt{avg_pool} \mid \texttt{sep_conv} \mid \texttt{depth_conv} \mid \texttt{conv} \mid \texttt{zero} \quad .
\end{aligned}
\tag{8}
$$

Mobile-net search space

Factorized hierarchical search spaces, e.g., the Mobile-net search space [32], 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) [56], 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 [57]. Consequently, we can express this search space as follows:

$$
\begin{aligned}
\text{MACRO} &::= \texttt{Linear}(\text{BLOCK, BLOCK, BLOCK}) \\
\text{BLOCK} &::= \texttt{Block}(\text{CONV, KSIZE, SERATIO, SKIP, FSIZE, \#LAYERS}) \\
\text{CONV} &::= \texttt{conv} \mid \texttt{dconv} \mid \texttt{mbconv} \\
\text{KSIZE} &::= \texttt{3} \mid \texttt{5} \\
\text{SERATIO} &::= \texttt{0} \mid \texttt{0.25} \\
\text{SKIP} &::= \texttt{pooling} \mid \texttt{id_residual} \mid \texttt{no_skip} \\
\text{FSIZE} &::= \texttt{0.75} \mid \texttt{1.0} \mid \texttt{1.25} \\
\text{\#LAYERS} &::= \texttt{-1} \mid \texttt{0} \mid \texttt{1} \quad ,
\end{aligned}
\tag{9}
$$

where `conv`, `donv` and `mbconv` correspond to convolution, depthwise convolution, and mobile inverted bottleneck convolution [57], respectively.

Hierarchical random graph generator search space

The hierarchical random graph generator search space [9] consists of three hierarchical levels of random graph generators (i.e., `Watts-Strogatz` [58] and `Erdõs-Rényi` [59]). 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:

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

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.

I 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 Sec. 3.

[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 1 Bayesian Optimization algorithm [60].

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

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

I.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 [60].

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 [61]. The general procedures of BO is summarized in Algorithm 1.

We adopted the widely used acquisition function, expected improvement (EI) [62], 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 [63] which uses the predictive posterior of the surrogate model to assign hallucinated function values $\{\tilde{f}_p\}_{p\in\{1,\ ...,\ P\}}$ to the P candidate points with pending evaluations $\{\tilde{\mathbf{x}}_p\}_{p\in\{1,\ ...,\ P\}}$ and perform next BO recommendation in the batch by pseudo-augmenting the observation data with $\tilde{\mathcal{D}}_p = \{(\tilde{\mathbf{x}}_p, \tilde{f}_p)\}_{p\in\{1,\ ...,\ P\}}$, 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.

Algorithm 3 Weisfeiler-Lehman subtree kernel computation [18].

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 $h = 1, \dots H$ **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 $\mathcal{H}$

I.2 Weisfeiler-Lehman kernel

Inspired by Ru et al. [17], we adopted the Weisfeiler-Lehman (WL) graph kernel [18] 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. [17] 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 (Sec. 5 and K), we have found stronger neural architectures by incorporating the hierarchical information in the kernel design, which provides experimental support for above arguments.

I.3 Evolutionary operations in detail

For the evolutionary operations, we adopted ideas from grammar-based genetic programming [64, 65]. In the following, we will show how these evolutionary operations manipulate algebraic terms, e.g.,

$$\texttt{Linear}(\texttt{Residual}(\texttt{conv, id, conv}), \texttt{Residual}(\texttt{conv, id, conv}), \texttt{fc}) \quad , \tag{11}$$

from the search space

$$\text{S} \; ::= \texttt{Linear}(\text{S, S, S}) \mid \texttt{Residual}(\text{S, S, S}) \mid \texttt{conv} \mid \texttt{id} \mid \texttt{fc} \quad , \tag{12}$$

to generate evolved algebraic terms. Fig. 1 shows how we can derive the algebraic term in Eq. 11 from the search space in Eq. 12. For mutation operations, we first randomly pick a subterm of the algebraic term, e.g., $\texttt{Residual}(\texttt{conv, id, conv})$. Then, we randomly sample a new subterm with the same nonterminal symbol S as start symbol, e.g., $\texttt{Linear}(\texttt{conv, id, fc})$, and replace the previous subterm, yielding

$$\texttt{Linear}(\texttt{Linear}(\texttt{conv, id, fc}), \texttt{Residual}(\texttt{conv, id, conv}), \texttt{fc}) \quad . \tag{13}$$

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

$$\texttt{Linear}(\texttt{Residual}(\texttt{conv}, \texttt{id}, \texttt{conv}), \texttt{Residual}(\texttt{conv}, \texttt{id}, \texttt{conv}), \texttt{fc}) \quad . \tag{14}$$

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.

J Extended related work

Neural Architecture Search Neural Architecture Search (NAS) aims to automatically discover architectural patterns (or even entire architectures) [66]. Previous approaches, e.g., used reinforcement learning [19, 20], evolution [21], gradient descent [22], or Bayesian Optimization (BO) [17, 23, 24]. To enable the effective use of BO on graph-like inputs for NAS, previous works have proposed to use a GP with specialized kernels [17, 23], encoding schemes [24, 25], or graph neural networks as surrogate model [26–28]. 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 [29] with a fixed macro architecture while only few works considered more expressive hierarchical search spaces [4, 30, 32]. The latter works considered hierarchical assembly [30], combination of a cell- and network-level search space [4, 31], evolution of network topologies [33], factorization of the search space [32], parameterization of a hierarchy of random graph generators [9], a formal language over computational graphs [34], or a hierarchical construction of TensorFlow programs [35]. 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 [33, 67, 68]. Other works proposed approaches based on string rewriting systems [36, 37], cellular (or tree-structured) encoding schemes [38–41], hyperedge replacement graph grammars [42, 43], attribute grammars [44], CFGs [45–52], or And-Or-grammars [53]. 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.

K Details for Sec. 5

In this section, we report implementation details (Sec. K.2) as well as dataset details (Sec. K.3). We also present the search results and conduct an analyses on the architectures observed during all of our search runs (Sec. K.5).

K.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 [54] 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:

$$
\begin{aligned}
\text{D2} &::= \texttt{Linear3}(\text{D1, D1, D0}) \mid \texttt{Linear3}(\text{D0, D1, D1}) \mid \texttt{Linear4}(\text{D1, D1, D0, D0}) \\
\text{D1} &::= \texttt{Linear3}(\text{C, C, D}) \mid \texttt{Linear4}(\text{C, C, C, D}) \mid \texttt{Residual3}(\text{C, C, D, D}) \\
\text{D0} &::= \texttt{Linear3}(\text{C, C, CL}) \mid \texttt{Linear4}(\text{C, C, C, CL}) \mid \texttt{Residual3}(\text{C, C, CL, CL}) \\
\text{D} &::= \texttt{Linear2}(\text{CL, down}) \mid \texttt{Linear3}(\text{CL, CL, down}) \mid \texttt{Residual2}(\text{C, down, down}) \\
\text{C} &::= \texttt{Linear2}(\text{CL, CL}) \mid \texttt{Linear3}(\text{CL, CL}) \mid \texttt{Residual2}(\text{CL, CL, CL}) \\
\text{CL} &::= \texttt{Cell}(\text{OP, OP, OP, OP, OP, OP}) \\
\text{OP} &::= \texttt{zero} \mid \texttt{id} \mid \text{BLOCK} \mid \texttt{avg_pool} \\
\text{BLOCK} &::= \texttt{Linear3}(\text{ACT, CONV, NORM}) \\
\text{ACT} &::= \texttt{relu} \mid \texttt{hardswish} \mid \texttt{mish} \\
\text{CONV} &::= \texttt{conv1x1} \mid \texttt{conv3x3} \mid \texttt{dconv3x3} \\
\text{NORM} &::= \texttt{batch} \mid \texttt{instance} \mid \texttt{layer} \quad .
\end{aligned}
\tag{15}
$$

See App. C for the terminal vocabulary of topological operators and primitive computations. The productions with the nonterminals $\{\text{D2, D1, D0, D}\}$ define the spatial resolution flow and together with $\{\text{C}\}$ define the macro architecture containing possibly multiple branches. The productions for $\{\text{CL, OP}\}$ construct the NAS-Bench-201 cell and $\{\text{BLOCK, ACT, CONV, NORM}\}$ 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 App. F 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.

K.2 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., [17]). 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.

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

Dataset	License	URL
CIFAR-10 [69]	MIT	`https://www.cs.toronto.edu/~kriz/cifar.html`
CIFAR-100 [69]	MIT	`https://www.cs.toronto.edu/~kriz/cifar.html`
ImageNet-16-120 [70]	MIT	`https://patrykchrabaszcz.github.io/Imagenet32/`
CIFARTile [71]	GNU	`https://github.com/RobGeada/cvpr-nas-datasets`
AddNIST [71]	GNU	`https://github.com/RobGeada/cvpr-nas-datasets`

K.3 Dataset details

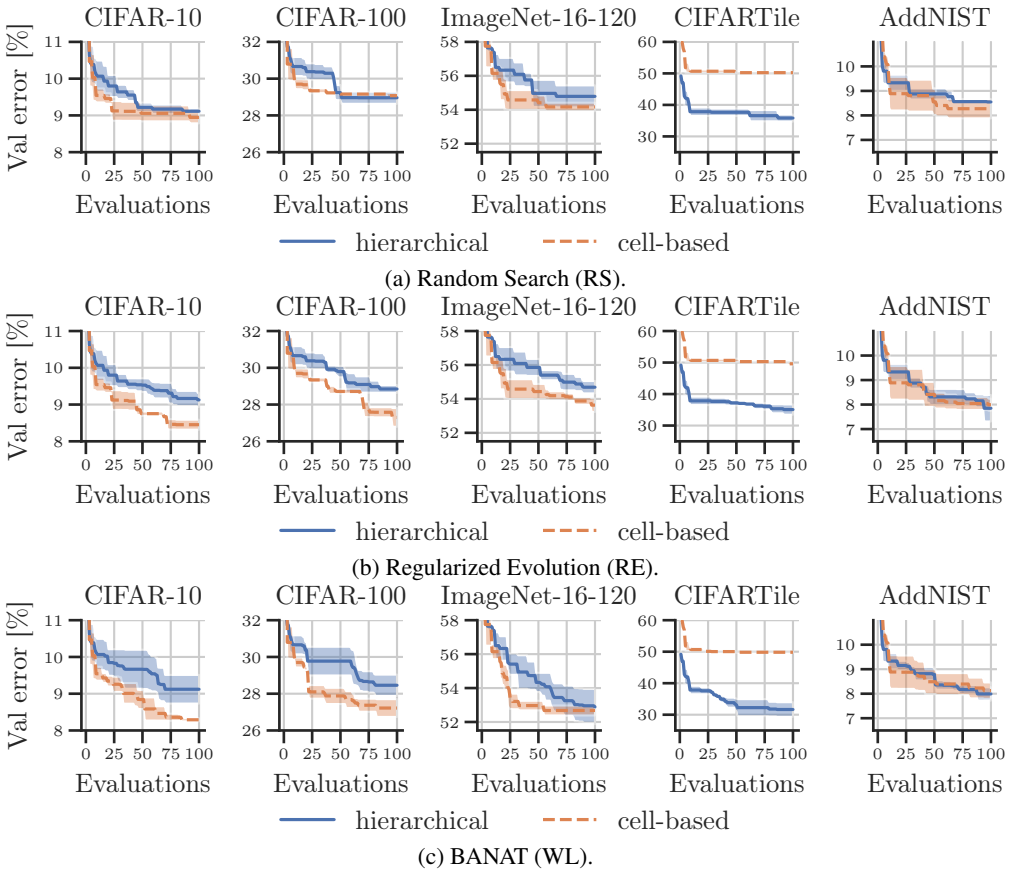
In Tab. 2, we provide the licenses for the datasets used in our experiments. For training of architectures on CIFAR-10, CIFAR-100 [69], and ImageNet-16-120 [70], we followed the dataset splits and training protocol of NAS-Bench-201 [54]. For CIFAR-10, we split the original training set into a new training set with 25k images and validation set with 25k images following [54]. 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 [71].

K.4 Evaluation details

We compared four different search strategies, i.e., BANAT, Random Search (RS), Regularized Evolution (RE), and BANAT (WL) [17]. For implementation details of the search strategies, please refer to App. K.2. 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 [69], ImageNet-16-120 [70], CIFARTile, and AddNIST [71]. We provide further dataset details in App. K.3. 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 and Yang [54]. We trained architectures with SGD with learning rate of 0.1, Nesterov momentum of 0.9, weight decay of 0.0005 with cosine annealing [72], 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 [71]: 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.

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) [17]. We ran 20 trials over the seeds $\{0,\ 1,\ ...,\ 19\}$ 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.



(a) Random Search (RS).

(b) Regularized Evolution (RE).

(c) BANAT (WL).

Figure 5: 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).

K.5 Further search results and analyses

Supplementary to Fig. 2 (top), Fig. 5 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.

We report the test errors of our best found architectures in Tab. 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 [55]) (**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.

Table 3: Test errors (and ± 1 standard error) of popular baseline architectures (e.g., ResNet [73] and EfficientNet [2] 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 and Yang [54].
(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 [73]	6.49 ± 0.24 (32)		27.1 ± 0.67 (110)		53.67 ± 0.18 (56)		57.8 ± 0.57 (18)		7.78 ± 0.05 (34)	
Best EfficientNet [2]	11.73 ± 0.1 (B0)		35.17 ± 0.42 (B6)		77.73 ± 0.29 (B0)		61.01 ± 0.62 (B0)		13.24 ± 0.58 (B1)	
NAS-Bench-201 oracle†	5.63		26.49		52.69		-		-	
RS	6.39 ± 0.18	6.77 ± 0.1	28.75 ± 0.57	29.49 ± 0.57	54.83 ± 0.78	54.7 ± 0.82	$\mathbf{52.72 \pm 0.45}$	40.93 ± 0.81	7.82 ± 0.36	8.05 ± 0.29
RE	$\mathbf{5.76 \pm 0.17}$	6.88 ± 0.24	27.68 ± 0.55	30.0 ± 0.32	53.92 ± 0.6	55.39 ± 0.54	52.79 ± 0.59	40.99 ± 2.89	$\mathbf{7.69 \pm 0.35}$	7.56 ± 0.69
BANAT (WL)	$\mathbf{5.68 \pm 0.11}$	6.98 ± 0.5	27.66 ± 0.18	28.7 ± 0.64	53.67 ± 0.39	53.47 ± 0.86	52.81 ± 0.27	35.75 ± 1.58	7.86 ± 0.41	8.2 ± 0.37
BANAT	$\mathbf{5.68 \pm 0.11}$	$\mathbf{6.0 \pm 0.16}$	27.66 ± 0.18	27.57 ± 0.46	53.67 ± 0.39	53.43 ± 0.61	52.81 ± 0.27	$\mathbf{32.28 \pm 2.39}$	7.86 ± 0.41	$\mathbf{6.09 \pm 0.34}$
BANAT (best)	5.64 ± 0.14	5.65 ± 0.09	27.03 ± 0.23	27.63 ± 0.2	53.54 ± 0.43	52.78 ± 0.23	53.18 ± 0.91	30.33 ± 0.77	8.04 ± 0.45	6.33 ± 0.59

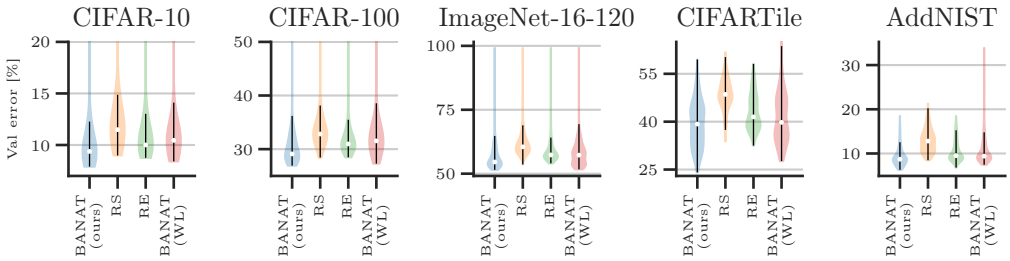


Figure 6: Density estimates for the validation error of all architecture candidates proposed by the search strategies (i.e., BANAT, RS, RE, and BANAT (WL)) and across datasets (i.e., CIFAR-10/100, ImageNet-16-120, CIFARTile, AddNIST) from our experiments in Sec. 5.

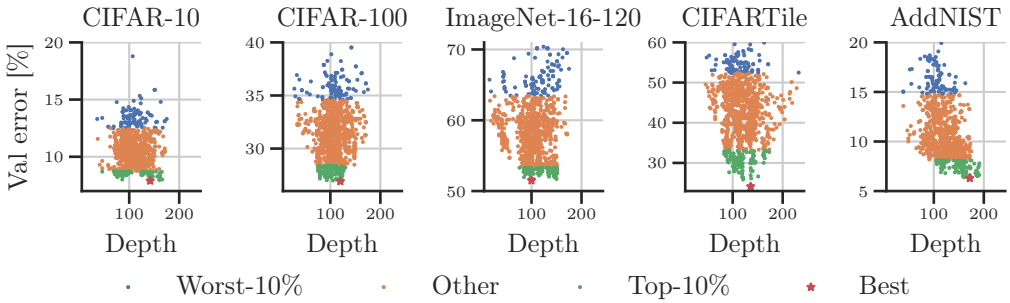
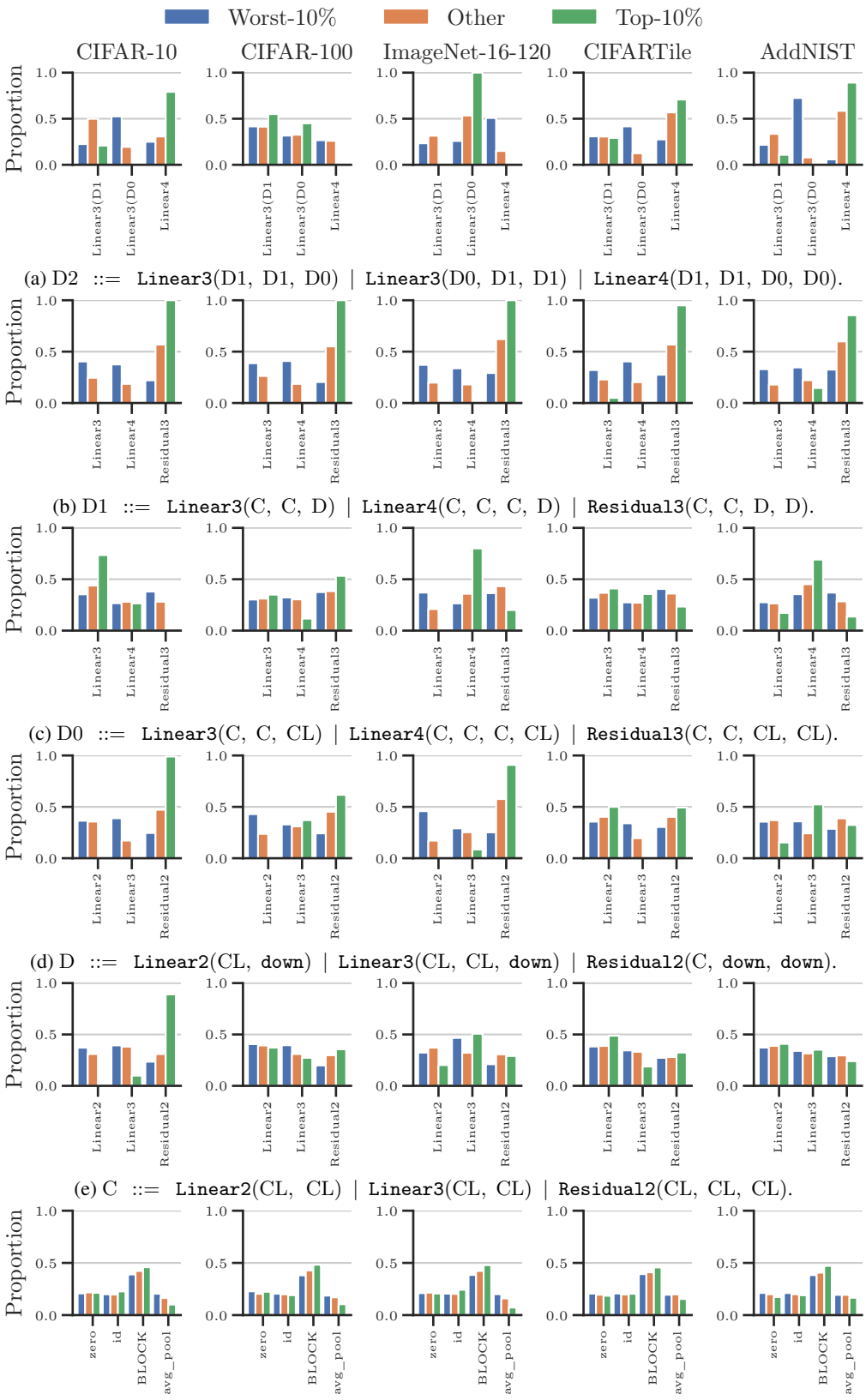


Figure 7: Validation error over maximal depth of all architecture candidates proposed by the search strategies (i.e., BANAT, RS, RE, and BANAT (WL)) and across datasets (i.e., CIFAR-10/100, ImageNet-16-120, CIFARTile, AddNIST) from our experiments in Sec. 5.

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 Sec. 5. This provides a better view for whether search strategies are exploring well-performing architectures or wasting computational resources on low-performing architectures. Fig. 6 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 7 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, Fig. 8 and Fig. 9 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.



(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`.

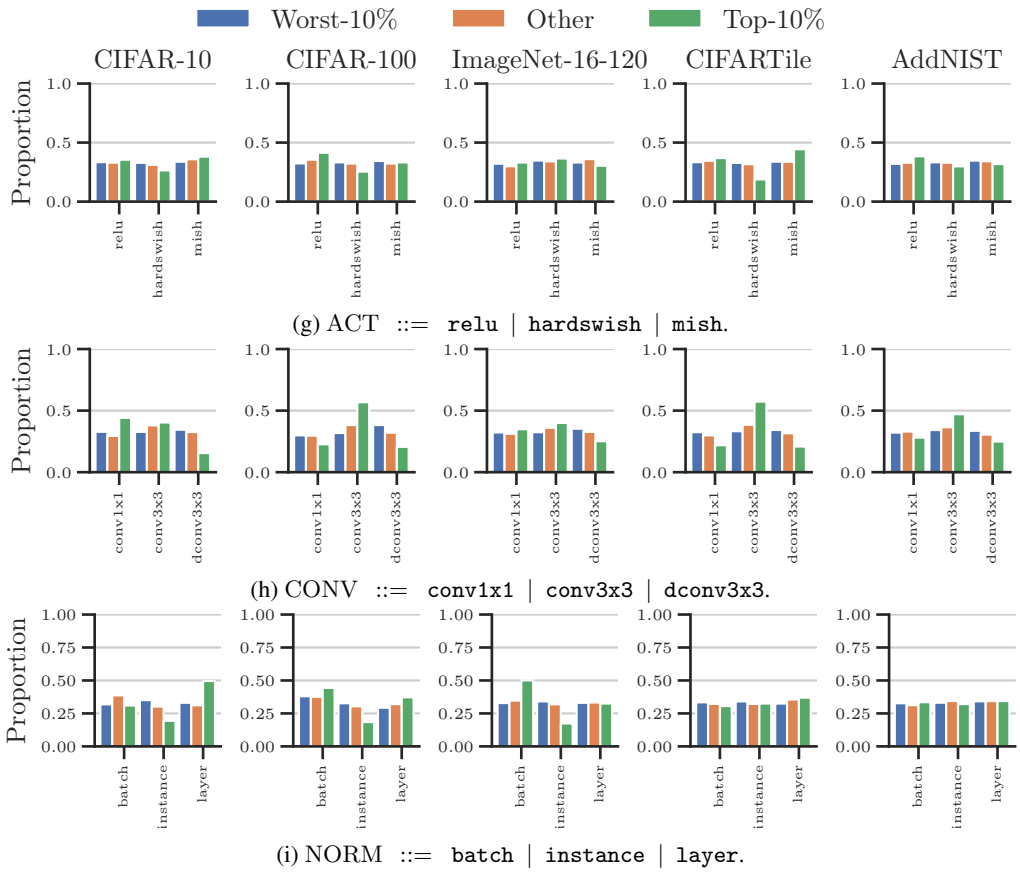
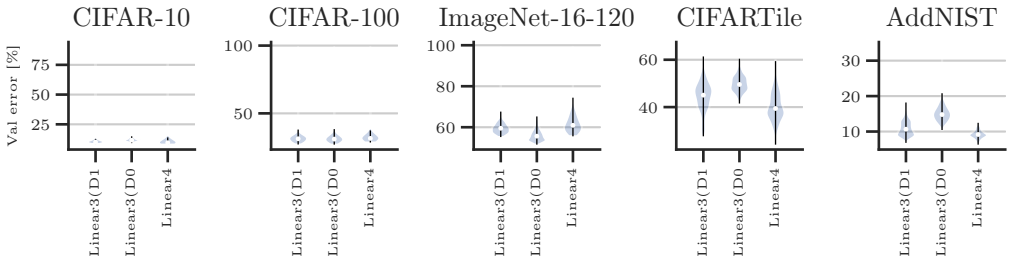


Figure 8: Comparison of the proportion of production rules in the worst-10% (blue), top-10% (green) and other (orange) neural architectures from our experiments in Sec. 5.

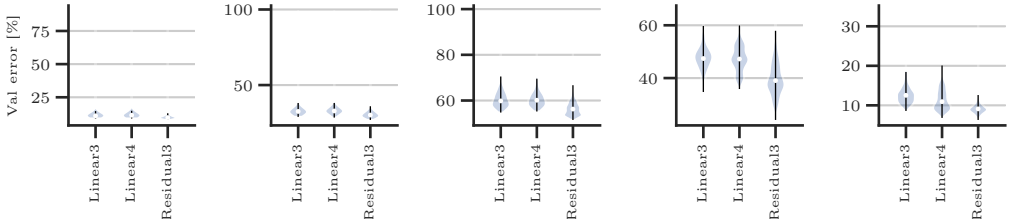
Best architectures Below we report the best found architecture per dataset on the hierarchical NAS-Bench-201 search space (App. K.1) for each dataset. Figure 10 provides a graphical summary of the best architectures.

CIFAR-10 (mean test error 5.65 %, #params 2.204 MB, FLOPs 127.673 M):

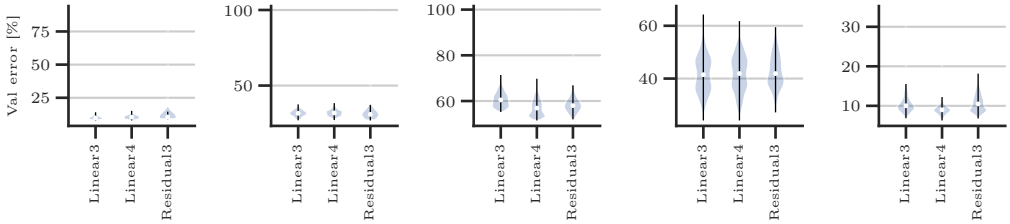
Linear4(Residual3(Residual2(Cell(id, zero, Linear1(Linear3(hardswish, conv1x1, layer)), Linear1(Linear3(hardswish, conv3x3, layer)), zero, Linear1(Linear3(mish, conv3x3, instance))), Cell(Linear1(Linear3(relu, dconv3x3, layer)), id, avg_pool, Linear1(Linear3(relu, dconv3x3, layer)), id, zero), Cell(zero,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



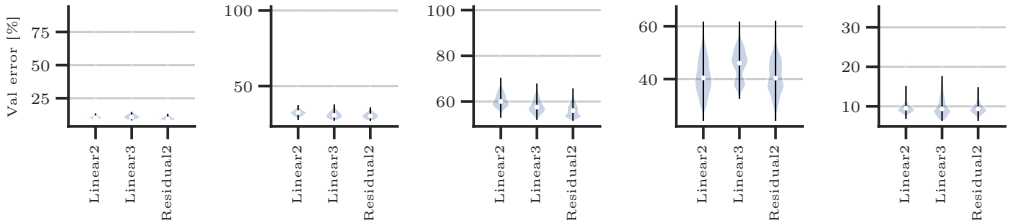
(a) D2 ::= `Linear3`(D1, D1, D0) | `Linear3`(D0, D1, D1) | `Linear4`(D1, D1, D0, D0).



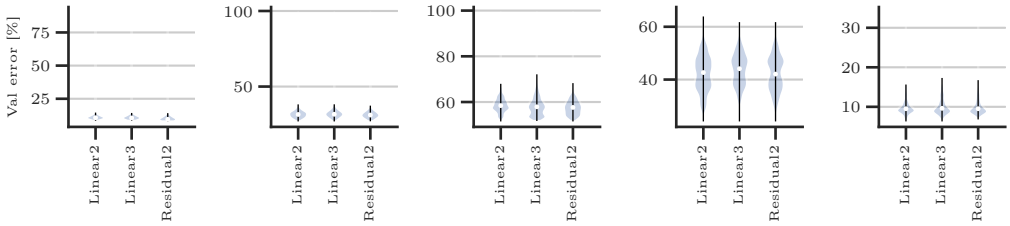
(b) D1 ::= `Linear3`(C, C, D) | `Linear4`(C, C, C, D) | `Residual3`(C, C, D, D).



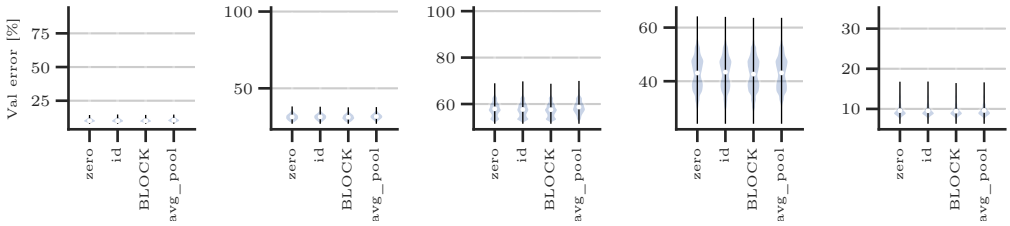
(c) D0 ::= `Linear3`(C, C, CL) | `Linear4`(C, C, C, CL) | `Residual3`(C, C, CL, CL).



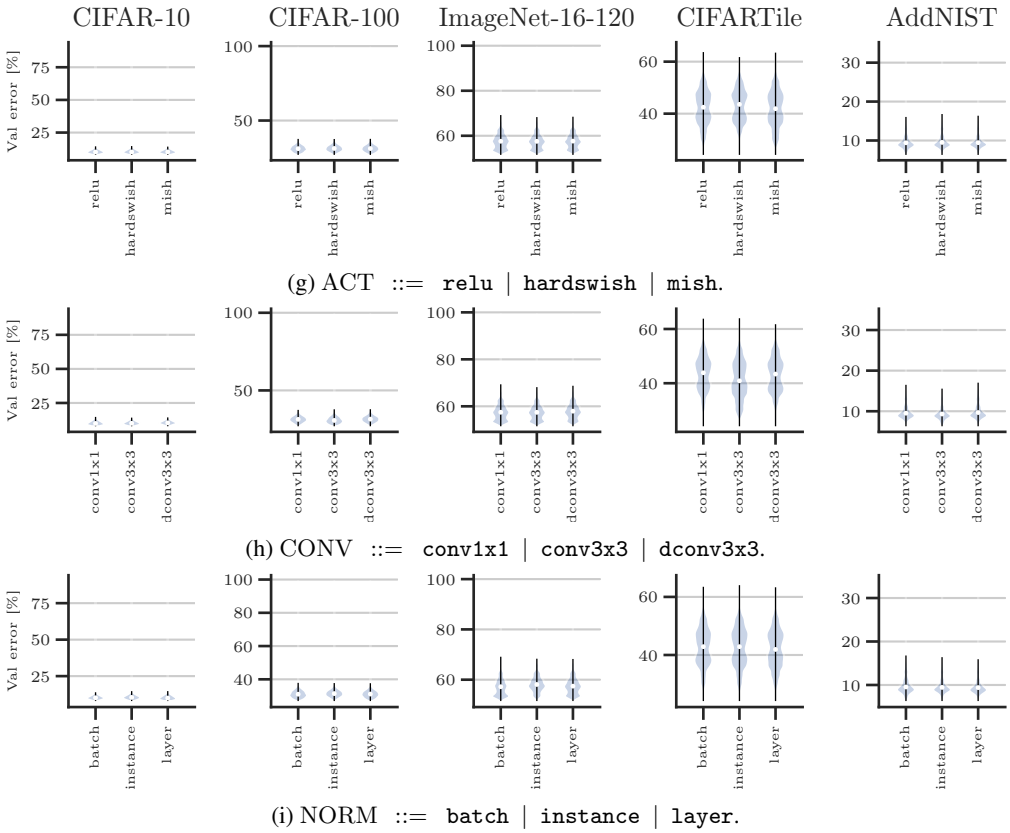
(d) D ::= `Linear2`(CL, `down`) | `Linear3`(CL, CL, `down`) | `Residual2`(C, `down`, `down`).



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



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



(g) ACT ::= `relu` | `hardswish` | `mish`.

(h) CONV ::= `conv1x1` | `conv3x3` | `dconv3x3`.

(i) NORM ::= `batch` | `instance` | `layer`.

Figure 9: Marginalized performance of every production rule in our hierarchical NAS-Bench-201 search space from Sec. 5.

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, 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 $0.962\,\mathrm{MB}$, FLOPs $115.243\,\mathrm{M}$):

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 $0.626\,\mathrm{MB}$, FLOPs $23.771\,\mathrm{M}$):

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 $372.114\,\mathrm{M}$):

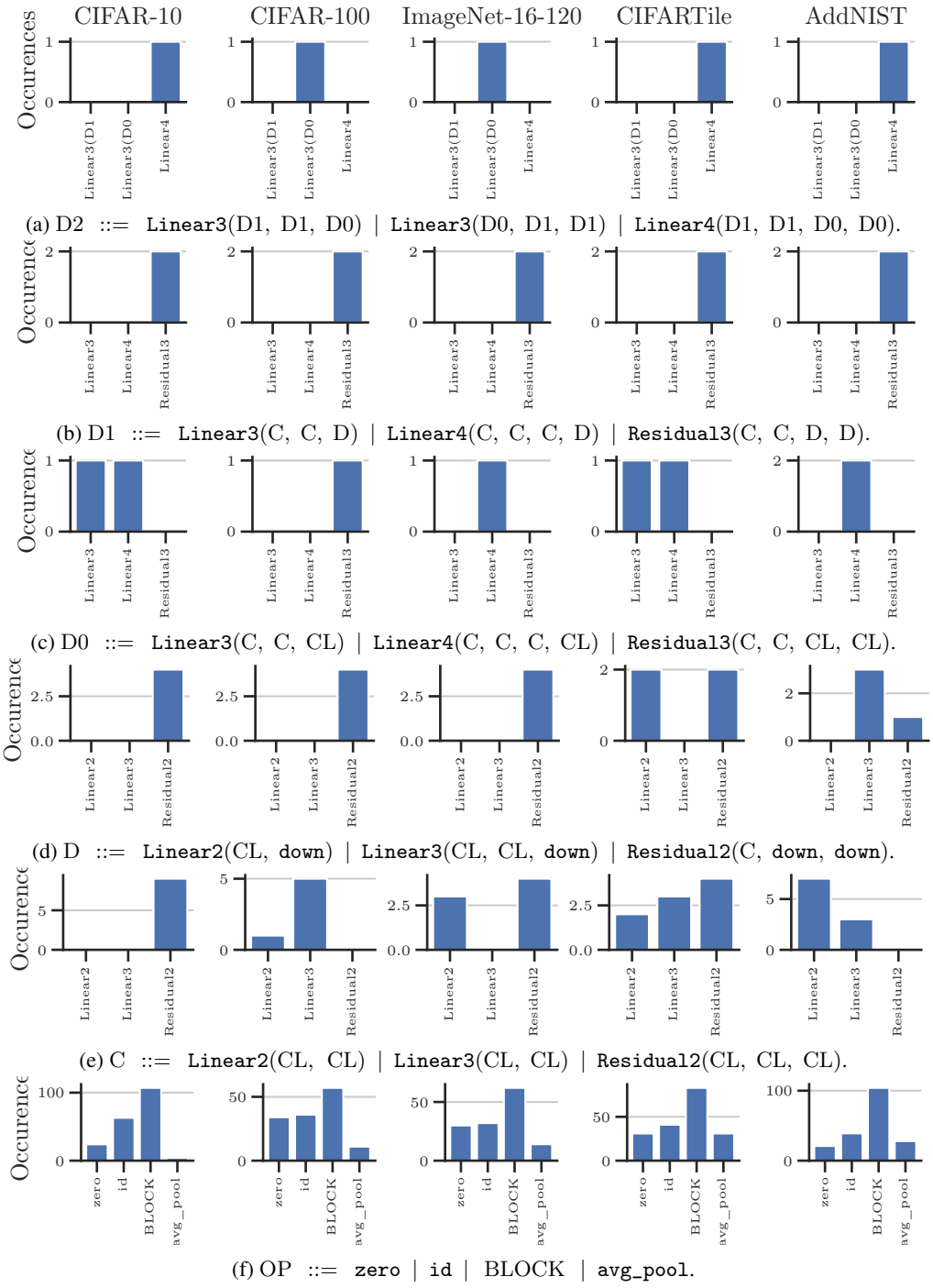
Linear4(Residual3(Residual2(Cell(Linear3(hardswish, conv3x3, instance), id, zero, Linear3(relu, dconv3x3, instance), Linear3(mish, conv1x1, instance), avg_pool), Cell(avg_pool, avg_pool, id, zero, Linear3(hardswish, conv3x3, batch), avg_pool), Cell(Linear3(relu, dconv3x3, instance), zero, id, Linear3(relu,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

Q3 Does leveraging the hierarchical information improve performance?



(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`.

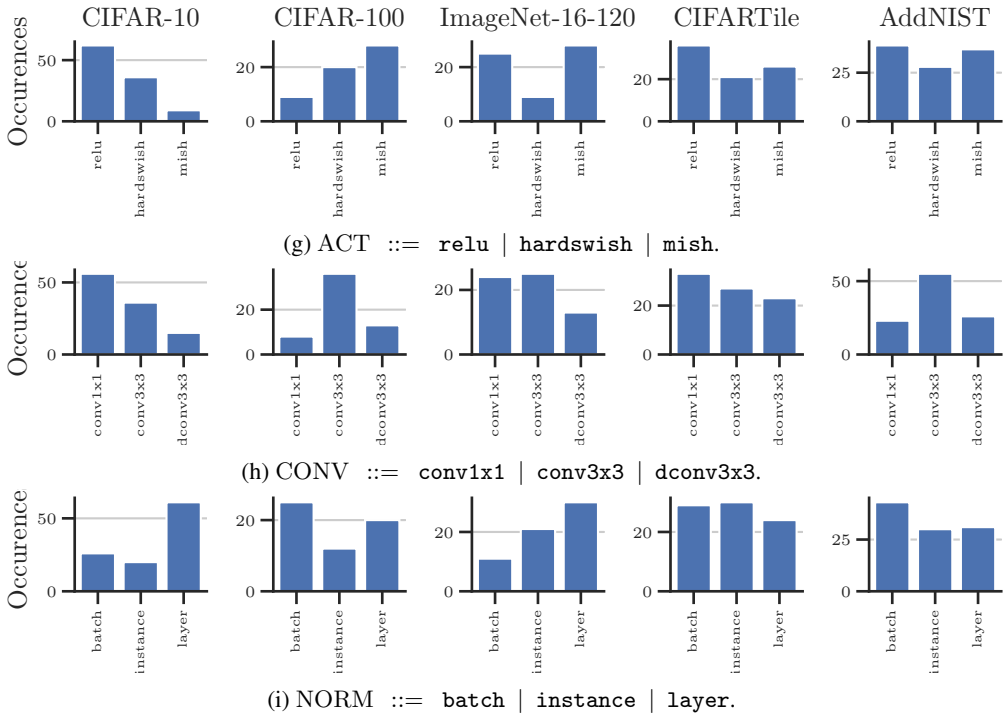


Figure 10: Summary of the distribution of topological operators and primitive operations of the best architectures on the hierarchical NAS-Bench-201 search space.

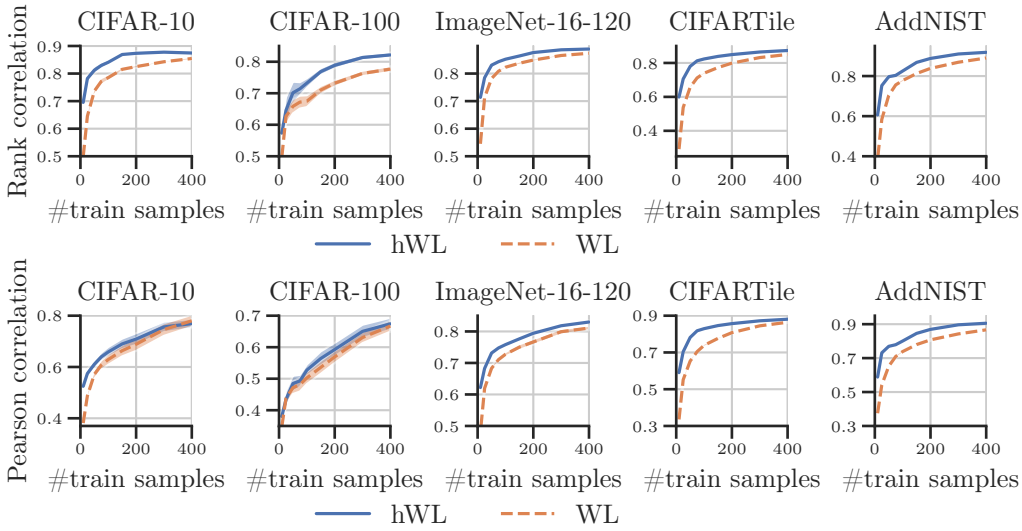


Figure 11: Mean Spearman's rank correlation (top) and Pearson correlation (bottom) with ± 1 standard error achieved by a GP with our hierarchical WL kernel (hWL) or without it (WL).