Neural Architecture Search as Sparse Supernet

Yan Wu\textsuperscript{1}, Aoming Liu\textsuperscript{1}, Zhiwu Huang\textsuperscript{1}, Siwei Zhang\textsuperscript{1}, Luc Van Gool\textsuperscript{1, 2}

\textsuperscript{1}ETH Zurich, Switzerland, \textsuperscript{2}KU Leuven
\{wuyan, aoliu, szhang\}@student.ethz.ch,
\{zhiwu.huang, vangool\}@vision.ee.ethz.ch

Abstract

This paper aims at enlarging the problem of Neural Architecture Search from Single-Path and Multi-Path Search to automated Mixed-Path Search. In particular, we model the new problem as a sparse supernet with a new continuous architecture representation using a mixture of sparsity constraints, i.e., Sparse Group Lasso. The sparse supernet is expected to automatically achieve sparsely-mixed paths upon a compact set of nodes. To optimize the proposed sparse supernet, we exploit a hierarchical accelerated proximal gradient algorithm within a bi-level optimization framework. Extensive experiments on CIFAR-10, CIFAR-100, Tiny ImageNet and ImageNet demonstrate that the proposed methodology is capable of searching for compact, general and powerful neural architectures.

1 Introduction

Deep learning has proven its superiority over manual feature engineering by learning representations in conjunction with statistical models in an end-to-end manner. However, neural network architectures are typically designed by experts in a tedious and ad hoc fashion. Neural Architecture Search (NAS) has been suggested as the path forward for alleviating the network engineering pain by automatically optimizing architectures that are superior to hand-designed ones. The automatically searched architectures perform competitively in computer vision tasks such as image classification [45, 26, 46, 27, 30, 9, 29, 5, 36, 43, 40], object detection [46], semantic segmentation [24, 7] and image generation [14].

As one of the most popular NAS families, one-shot NAS generally models the architecture search problem as a one-shot training process of an over-parameterized supernet that comprises all architectures (paths). From the supernet, either Single-Path or Multi-Path architecture can be optimized. For the Single-Path Search, most algorithms require a rigid structure on the searched architectures. For instance, [27, 12, 25] search for a computation cell as the backbone block of the final architecture. Based on the modeling of directed acyclic graph, the cell is typically required to have two input nodes and a single output node, each of which corresponds to a feature map, and the associated edge between each pair of nodes should have one single operation like convolution, max pooling, zero. The requirement results in a single neural architecture, where each feature map is processed by a single operation. On the other hand, while Multi-Path architecture search like [12, 11] is more flexible to optimize multiple paths, they require to fix the number of paths in advance. Moreover, both the existing Single-Path and Multi-Path Search methods have to manually fix the node number.

In this paper, we target for a more automated NAS which can automatically optimize the mixture of paths as well as a changeable set of nodes. In other words, the target of automated Mixed-Path Architecture Search is to reduce unnecessary constraints on the structure of the searched architecture. In theory, enforcing less constraints will lead to a better optimization for automated architecture.

\textsuperscript{*}Equal contribution

Preprint. Under review.
search. For this purpose, we model the automated NAS problem as a one-shot searching process of an sparse supernet, which consists of sparsely-mixed paths and nodes without loss of network power, e.g., classification ability. In particular, we exploit a new continuous architecture representation with a Sparse Group Lasso constraint to achieve the sparse supernet. As a result, the supernet is not only able to produce diverse mixed-paths between different pairs of nodes, but also automatically removes some useless nodes. The more general model however makes the optimization much more challenging due to the complex bi-level optimization with a non-differentiable sparsity constraint, which cannot be optimized by traditional network optimization algorithms well. To address this challenging issue, we propose a hierarchical accelerated proximal gradient algorithm that is capable of treating the mixed sparsity constraint within the bi-level optimization.

In summary, this paper brings several innovations to the domain of NAS as follows:

- We suggest a new problem of Mixed-Path Neural Architecture Search where the path and node structure are automatically derived.
- We model the problem as a sparse supernet using a new continuous architecture representation with a mixture of sparsity constraints.
- We propose a hierarchical accelerated proximal gradient algorithm to optimize the supernet search with the mixed sparsity constraints.
- We study that the searched Mixed-Path architectures are compact, general and powerful for standard NAS benchmarks.

2 Problem Statement

Neural Architecture Search aims at searching for computation cells as the basic building block of the final architecture. In general, each architecture cell can be formulated as a directed acyclic graph (DAG) as shown in Fig.1 (a) where each node represents a feature map in neural networks, and each directed edge is a mixture of operations that transform the tail node to the head node. As a consequence, the output of each intermediate node is a sum of incoming feature maps from its predecessors. The DAG modeling enables the training of an over-parameterized supernet that stacks multiple basic cells. The optimal architecture is then derived or searched from the supernet with the following three strategies.

**Single-Path Architecture Search** methods generally search for only one operation on each node pair with fixed edge amounts in each cell as shown in Fig.1 (b). In order to make the single path selection from a given supernet, they commonly first optimize the mixture of all associated operations, and finally choose those with the highest contribution to the supernet. As one of the most representative Single-Path Search methods, Differentiable Architecture Search (DARTS) [27] optimizes the mixture of operations within supernet using softmax combination. For each edge, the operation with largest softmax weight was selected. For each node, two input edges was selected by comparing each edge’s largest operation weight. The rigid requirement on final architecture highly reduces the search space, such that the optimization process has a high potential to be stuck at a local minimum.
**Multi-Path Architecture Search** searches and compares multiple paths between any nodes (Fig. 1 (c)), which is inspired by Multi-Path feature aggregations such as Inception networks [34] and ResNeXt [37]. While Multi-Path supernet might take benefits from aggregations, comparing multiple paths is not as straightforward as comparing single paths. To address this issue, [11] samples multiple paths during search, while [10] uses Fourier analysis of Boolean functions with Fourier basis representing multiple paths. Nevertheless, the Multi-Path Search approach still requires a strong prior knowledge about the aggregation intensity (i.e., path number) in advance of search. Furthermore, enforcing the same number of operations for each pair of nodes is very likely to reach a locally optimal architecture.

**Mixed-Path Architecture Search** is hence suggested for the exploration of a more general search space to avoid the human intervene as much as possible. For this purpose, we consider to enlarge the domain of Neural Architecture Search by relaxing the constraints on the network structure. In particular, the supernet is merely required to learn a complete and compact neural architecture, without any more rigid constraints on the node and path structure. In other words, it should be trained to automatically derive an optimal node and path structure as compact as possible without loss of network ability for specific tasks like image classification. The suggested new problem is conceptually illustrated in Fig. 1 (d). In comparison to Single-Path Search and Multi-Path Search, Mixed-Path Search dramatically increases the architecture search space, and thus leading to a much more challenging NAS problem.

## 3 Sparse Supernet

Our Mixed-Path Architecture Search starts from an over-parameterized supernet and aims at deriving an compact and optimal neural architecture. With the target of automatically selecting useful operations and nodes within the supernet, we are inspired by the prevailing sparsity regularization in linear regression which can act as an automated feature selection mechanism. We thereby consider to introduce a sparse constraint to our supernet to select meaningful feature maps automatically. With imposed sparsity constraint, we enable an automated sparse Mixed-Path Architecture Search.

The supernet is designed as a stack of repetitive cells, and each cell is formulated as a DAG cell. In particular, the mixture of operations on each edge is formulated in a "regression-like" way. Instead of employing the widely-used softmax combination and its variants, such as Gumbel softmax[6], we formulate the edge $e_{ij}$ between node $x_i$ and $x_j$ as a linear combination of operations and feature map derived from each operation $o$.

The output feature map of intermediate node is now a scaled linear combination of various feature maps from different predecessors with different operations, i.e.,

$$ x_j = \sum_{i<j} \sum_{o \in O} A_{ij}^o o(x_i), A_{ij}^o \in \mathbb{R} $$

To relax the structure constraints on both the number of nodes and paths per edge, we aim at achieving the node sparsity as well as the operation sparsity. Sparse Group Lasso (SGL) regularization [32] meets our expectation exactly which allows for both element sparsity and group sparsity. In a DAG with $N$ intermediate nodes, for each node $x_j$, we group weight factors for all incoming feature maps $A_{ij}^o$, where $i < j, o \in O$ as $A_{[j]}$. Mathematically, the full objective function can be derived as:

$$ L(w, A) = l(w, A) + \Omega_{SGL}(A) = l(w, A) + \lambda \alpha ||A||_1 + \lambda (1 - \alpha) \sum_{n=1}^{N} \sqrt{|A_{[n]}|} \cdot ||A_{[n]}||_2 $$

where $\Omega_{SGL}$ corresponds to the mixed sparsity regularization, $\lambda$ controls the strength of sparsity constraint, and $\alpha$ controls the balance between operation-wise sparsity and node-wise sparsity. By optimizing the network parameters $w$ and weight factors $A$ with the target function in Eq. 2, we can learn a sparse supernet adaptively during supernet training. Ideally, the final sparse supernet will be derived by removing the operations with weight zero and nodes with all zero incoming weights.

To jointly optimize the supernet and learn a sparse network structure, we target for solving the following bi-level optimization problem:

$$ \min_A \quad l_{train}(w^*(A), A) + \Omega_{SGL}(A) $$

subject to

$$ w^*(A) = \arg\min_w \quad l_{val}(w, A) $$
where the network weights $w$ and architecture weight factors $A$ are optimized on two separate train set and valid set to avoid architecture from overfitting to data.

4 Optimization

As $\ell_1$-norm term being convex while non-differentiable, the Sparse Group Lasso regularization term yields a more challenging optimization problem. Conventional stochastic gradient descent algorithms, such as SGD and Adam generally cannot work well. While some exiting works like [33, 18] have exploited blockwise descent algorithms to fit Sparse Group Lasso, it is non-trivial to apply their algorithms to the stochastic optimization setting. We thereby turn to the proximal methods [3] which is capable of solving the optimization problem with the non-differentiable term and enables us to learn some exact zero weights via soft-threshold. We propose a novel hierarchical proximal solution HAPG which is suitable for stochastic optimization and its improved version AdamHAPG, and we further appropriately incorporate these two methods into the bi-level optimization framework.

4.1 Hierarchical Proximal Optimization

Computing the proximal operator $\text{Prox}_{\Omega}(\cdot)$ associated with the regularization term $\Omega$ is to a key part of proximal method. The joint combination of $\ell_1$ and $\ell_1/\ell_2$ norm in Sparse Group Lasso brings much higher complexity to the direct proximal operator computing. Inspired by [3] that the Sparse Group Lasso norm is a special case of hierarchical norm [42], with $\ell_1$-norm of each individual weight factor being a child group of the $\ell_1/\ell_2$-norm, we derive the hierarchical proximal operator as a composition of $\ell_1$-norm and $\ell_1/\ell_2$-norm proximal operators:

$$\text{Prox}_\Omega(\cdot) = \text{Prox}_{\lambda_1(1-\alpha)||\cdot||_2} \circ \text{Prox}_{\lambda_1||\cdot||_1}(\cdot)$$

As for proximal algorithm, widely-used methods include ISTA and FISTA [4], and here we employ an efficiently reformulated Accelerated Proximal Gradient (APG) optimization scheme [17] which allows for the stochastic optimization setting. Accordingly, we propose a Hierarchical Accelerated Proximal Gradient (HAPG) algorithm tailored for the Sparse Group Lasso regularization:

$$z_t = A_{t-1} - \eta_t g_{t-1}$$

$$v_t = \text{Prox}_{\eta_1(1-\alpha)||\cdot||_2} \circ \text{Prox}_{\eta_1||\cdot||_1}(z_t) - A_{t-1} + u_{t-1} v_{t-1}$$

$$A_t = \text{Prox}_{\eta_1(1-\alpha)||\cdot||_2} \circ \text{Prox}_{\eta_1||\cdot||_1}(z_t) + u_t v_t$$

where $g_{t-1}$ represents the gradient, $\eta_t$ is the gradient step size and $u_t = \frac{t-2}{t+1}$. And the proximal operators can be derived as:

$$[\text{Prox}_{\eta_1(1-\alpha)||\cdot||_2}(z)]_i = \text{sgn}(z_i)(|z_i| - \eta_1 \alpha)_+$$

$$[\text{Prox}_{\eta_1||\cdot||_1}(z)]_n = \left(1 - \frac{\sqrt{|z_n|} \eta_1(1-\alpha)}{|z_n||z_n|_2}\right)_+ z_n$$

To further facilitate the optimization, we introduce the powerful Adam into the proposed HAPG framework and replace the gradient descent in Eq.6 with an Adam gradient update [19]. We should note that each weight factor gets an individual gradient step size in AdamHAPG, and we thereby make small adaptations when computing proximal operators. As for the $\ell_1$-norm proximal operator, we implement the proximal update using the corresponding step size for each weight, while for the $\ell_1/\ell_2$-norm proximal operator, we heuristically take the median value of step sizes for each group as an approximation and we experimentally show that it works properly for our problem.

4.2 Bi-level Optimization with Hierarchical Proximal Optimization

We incorporate our hierarchical proximal algorithms into the bi-level optimization framework to alternatively optimize the network parameters $\omega$ and architecture weight factor $A$. Particularly, we follow [27] to compute the gradient of architecture weight (i.e., $g_{t-1}$ in Eq.6):

$$g_t = \nabla_{A} l_{\text{val}}(w^*(A_t), A_t)$$

$$\approx \nabla_{A} l_{\text{val}}(w^*_t, A_t) - \gamma \nabla_{A,w} l_{\text{train}}(w_t, A_t) \nabla_{w} l_{\text{val}}(w^*_t, A_t)$$

$$\approx \nabla_{A} l_{\text{val}}(w^*_t, A_t) - \frac{\nabla_{A} l_{\text{train}}(w^*_t, A_t) - \nabla_{A} l_{\text{train}}(w_t, A_t)}{2\epsilon}$$
Mixed-Path Architecture Search as a supernet with the Sparse Group Lasso, which enables us to aim at deriving more compact and complete node and path structures. To this end, we model the architecture search is still limited to search with a fixed number of paths.

BayesNAS [44] exploits either \( \ell_1 \)-norm sparsity (with the same drawback with [41]) or group-level sparsity with a weighted Group Lasso constraint in the classic Bayesian leaning manner, leading to sparse node structures. However, their suggested Group Lasso constraint merely focuses on the sparsity on groups (i.e., nodes), and theoretically it is very likely to reach unsatisfactory sparsity on elements (i.e., paths). By comparison, our suggested Mixed-Path Architecture Search problem aims at deriving more compact and complete node and path structures. To this end, we model the Mixed-Path Architecture Search as a supernet with the Sparse Group Lasso, which enables us to go for a more compact structure of nodes and paths. Accordingly, we believe our work serves as.

5 Related Work

Network Pruning targets for reducing the model complexity by removing redundant network weights, neurons, layers, etc. Some network pruning works [17, 31, 22, 28, 35, 2] proposed to impose sparsity constraint on network weights or auxiliary scale factors so as to sparsify the networks. In particular, [31] applies the Sparse Group Lasso constraint to remove network neurons, weights and select active input features. However, the search space of network pruning is fundamentally different from Neural Architecture Search. Network pruning focuses on pruning the neurons, weights or layers, while NAS is expected to focus on pruning the connections between different layers, namely structural connections.

Neural Architecture Search with one-shot model generally aims at Single-Path architecture search[27, 5, 36, 23, 38, 8, 21]. For instance, DARTS [27] relaxes the search space to be continuous architecture parameter for each path using softmax and model weights and architecture parameters are optimized alternatively via gradient descent. Based on DARTS, improvements including progressive search [8], fair comparison with sigmoid function [12], early stopping [23] are proposed. In addition, ProxylessNAS [5] and FBNet [36] also achieve Single-Path Architecture Search with single-path sampling.

Multi-Path Architecture Search problem is clearly proposed and approached in MixPath[11], although its name is MixPath. Similar to ProxylessNAS, MixPath uses sampling to compare paths. But MixPath activates \( m \) paths each time while ProxylessNAS only activate a single path. A Shadow Batch Normalization is proposed to stabilize the training with Multi-Path activation. GreedyNAS[40] is also Multi-Path architecture search with activating multiple paths. In addition to MixPath and GreedyNAS, CoNAS [10] achieves Multi-Path Architecture Search with Fourier analysis of Boolean functions. It samples sub-graph from a pre-trained one-shot model and do Fourier analysis based on the sub-graphs’ performances. The Fourier coefficients are used to rank the multiple paths represented by the Fourier basis. Path amount of Fourier basis is controlled by its degree \( d \). Thus, Multi-Path architecture search is still limited to search with a fixed number of paths.

Few works approach the variants of our defined Mixed-Path Architecture Search. For instance, DSO-NAS[41] enforces the \( \ell_1 \)-norm sparsity constraint (i.e., Lasso) to independent architecture parameters, which can achieve sparsely-mixed paths but it overlooks the quest for sparse node structures especially when nodes are redundant initially (e.g., search with DARTS’ cell structure). BayseNAS [44] exploits either \( \ell_1 \)-norm sparsity (with the same drawback with [41]) or group-level sparsity with a weighted Group Lasso constraint in the classic Bayesian leaning manner, leading to sparse node structures. However, their suggested Group Lasso constraint merely focuses on the sparsity on groups (i.e., nodes), and theoretically it is very likely to reach unsatisfactory sparsity on elements (i.e., paths). By comparison, our suggested Mixed-Path Architecture Search problem aims at deriving more compact and complete node and path structures. To this end, we model the Mixed-Path Architecture Search as a supernet with the Sparse Group Lasso, which enables us to go for a more compact structure of nodes and paths. Accordingly, we believe our work serves as

\[
\text{Algorithm 1: Bi-level Optimization with Hierarchical Accelerated Proximal Gradient (HAPG)}
\]

Require: Supernet parameterized by \( \mathcal{A}_{i,j} \) for each operation \( o \) between nodes \( i, j \);

while not converged do
  \hspace{1cm} \textbf{Step 1:} Update architecture weights \( \mathcal{A} \) with HAPG given in Eq.6-10. Note that the gradient are computed with second order approximation given in Eq.13.
  \hspace{1cm} \textbf{Step 2:} Update \( \mathbf{w} \) by descending \( \nabla_{\mathbf{w}} l_{\text{train}}(\mathbf{w}, \mathcal{A}) \);
end

Ensure: Sparse supernet based on sparse architecture weights \( \mathcal{A} \).

where \( \mathbf{w}' = \mathbf{w} - \gamma \nabla_{\mathbf{w}} l_{\text{train}}(\mathbf{w}, \mathcal{A}), \mathbf{w} = \mathbf{w} \pm \epsilon \nabla_{\mathbf{w}} l_{\text{train}}(\mathbf{w}, \mathcal{A}) \) and \( \epsilon \) and \( \gamma \) are set to be small scalars as done in [27]. Eq.12 is derived by an one-step forward approximation, i.e., \( w^*(\mathcal{A}) \approx \mathbf{w}' = \mathbf{w} - \gamma \nabla_{\mathbf{w}} l_{\text{train}}(\mathbf{w}, \mathcal{A}) \) and Eq.13 follows the second-order approximation in [27]. Especially, when introducing the HAPG and AdamHAPG to the bi-level optimization framework, to stabilize training, we suggest a similar pathwise solution as done in [33] while with an incremental increase of regularization factor \( \lambda \) and we experimentally show the effectiveness of this progressive sparsifying solution. The complete optimization algorithm is presented in Alg.1.
Figure 2: Comparison between Lasso, Group Lasso and Sparse Group Lasso and comparison between different optimization methods, including SGD, Adam, HAPG and AdamHAPG. From left to right: the valid accuracy of derived sparse network, the number of selected input features, the number of remained inner neurons, the total sparsity percentage of network weights.

a valuable pioneer study for such a more general Mixed-Path Architecture Search problem using a promising hierarchical proximal bi-level optimization.

6 Evaluation

6.1 Network Pruning

As network pruning is close to and much easier than the NAS task, we use it to purely validate the superiority of Sparse Group Lasso (SGL) over Lasso and Group Lasso (GL), and further evaluate effectiveness of our HAPG and AdamHAPG. Following [31] that applies network pruning to select features and remove potential redundant weights and neurons, we implement classification task on DIGITS [1] and start with a fully connected network with two hidden layers (40 and 20 hidden neurons respectively). We flatten the 8×8 image into a 64-dim vector as the input features and sparsity constraint is applied on the network weights. Please refer to supplementary materials for detailed experiment settings.

SGL can be readily extended to Lasso and GL by setting $\alpha$ to 1 and 0 respectively. We first compare the performances of Lasso, GL and SGL with different regularization strength in Fig. 2. With the same optimization algorithm, SGL indeed outperforms Lasso and GL both in terms of group (features and neurons) sparsity and element (network weights) sparsity. Further, we evaluate the advantage of HAPG and AdamHAPG on the SGL problem when comparing with conventional SGD and Adam. With fixed $\alpha = 0.5$ while different regularization strength factor $\lambda$, the performance of sparse networks as well as neuron and weight sparsity levels are shown in Fig. 2. As we can expect, as $\lambda$ increasing, stronger sparsity regularization derives sparser network. With regularization strength factor $\lambda$ ranging from $10^{-5}$ to $10^{-3.7}$, the competitors achieve well-performed sparse networks with comparable validation accuracy. Whereas, in terms of sparsity, our proposed HAPG and AdamHAPG clearly outperform their counterparts Adam and SGD. In particular, AdamHAPG shows a clear superiority to reach a more compact structure and more powerful feature selection ability.

6.2 Neural Architecture Search

The experiments are performed on four datasets, CIFAR10/100 [20], Tiny-ImageNet-200∗, and ImageNet [13]. The direct architecture search are implemented on CIFAR10 and TinyImageNet, and we further transfer the derived architectures to CIFAR100 and ImageNet. In all the experiments, we use the official implementation of DARTS [27] as our backbone to implement the proposed NAS method with sparse supernet (SparseNAS). Following [27], we use the same search space, the same normal and reduction cell setup, stack the same number of cells, and apply basically the same search and training settings. For search with HAPG, we experimentally set $\alpha$ as 0.3, and increase $\lambda$ by 0.001 every epoch. The init learning rate for architecture weight factors is 0.025 and a cosine annealing learning rate decay is applied. For search with AdamHAPG, we select the optimal $\alpha$ as 0.5 and $\lambda$ increase step as 0.01. For more experimental details, please refer to the Appendix A.

Evaluation on CIFAR10/100 The architecture searched on CIFAR10 is evaluated on CIFAR10 and transfered to CIFAR100. The evaluation results are summarized in Table 1. We could see that performance of SparseNAS on CIFAR10 is better than other Mixed-Path Architecture search works,
Table 1: Performance Comparison on CIFAR10/100 (lower error rate is better).

| Architecture                  | Test Error (%) | Params (M) | Search Cost (GPU days) | Architecture Type |
|-------------------------------|----------------|------------|------------------------|-------------------|
| DenseNet-BC [16]              | 3.46           | 17.18      | 25.6                   | –                 |
| DARTS (first order) [27]      | 3.00 ± 0.14    | 17.76      | 3.3                    | 1.5 Single-Path   |
| DARTS (second order) [27]     | 2.76 ± 0.09    | 17.54      | 3.3                    | 4 Single-Path     |
| P-DARTS [8]                   | 2.50           | 16.55      | 3.4                    | 0.3 Single-Path   |
| DARTS$^{+}$ [23]              | 2.50 ± 0.11    | 16.28      | 3.4                    | 0.3 Single-Path   |
| MixPath-c [11]                | 2.60           | –          | 5.4                    | 0.25 Multi-Path   |
| CoNAS [10]                    | 2.62 ± 0.06    | –          | 4.8                    | 0.7 Multi-Path    |
| DSO-NAS-share [41]            | 2.84 ± 0.07    | –          | 3.0                    | 1 Mixed-Path      |
| BayesNAS + cutout [44]        | 2.81 ± 0.04    | –          | 3.4                    | 0.2 Mixed-Path    |
| SparseNAS + HAPG              | 2.73 ± 0.05    | 16.83      | 3.8                    | 1 Mixed-Path      |
| SparseNAS + AdamHAPG          | 2.69 ± 0.03    | 17.04      | 4.2                    | 1 Mixed-Path      |
| SparseNAS + AdamHAPG$^*$      | 2.50           | 16.79      | 3.5                    | 0.27 Mixed-Path   |

$^{†}$ Obtained by searching in a small search space.
$^{‡}$ Performance obtained by transferring architecture searched on CIFAR10 to CIFAR100.
$^{∗}$ Contribution orthogonal to SparseNAS, which can also be applied to improve SparseNAS.

Table 2: Transferability Comparison on ImageNet in the Mobile Setting.

| Architecture                  | Test Error (%) | Params (M) | Architecture Type |
|-------------------------------|----------------|------------|-------------------|
| Architecture                  | top-1 | top-5 | manual |
| Inception-v1 [34]             | 30.20 | 10.1  | 6.6               |
| MobileNet [15]                | 29.40 | 10.5  | 4.2               |
| DARTS [27]                    | 26.70 | 8.7   | 4.7               | Single-Path       |
| P-DARTS [8]                   | 24.40 | 7.4   | 4.9               | Single-Path       |
| MixPath [11]                  | 22.80 | 6.5   | 5.1               | Multi-Path        |
| DSO-NAS [41]                  | 26.20 | 8.6   | 4.7               | Mixed-Path        |
| BayesNAS [44]                 | 26.50 | 8.9   | 3.9               | Mixed-Path        |
| SparseNAS + HAPG              | 25.48 | 8.1   | 5.3               | Mixed-Path        |
| SparseNAS + AdamHAPG          | 24.67 | 7.6   | 5.7               | Mixed-Path        |

$^{**}$ Obtained by direct search on ImageNet.

and is comparable with DARTS 2nd-order. SparseNAS architecture performs better than DARTS when transferring to CIFAR100. Specifically, the architecture searched in the small search space performs comparable with state-of-the-art improved-DARTS works [8]. Note that contributions of [23, 8] are orthogonal to our contribution, and also possible to be applied to improve SparseNAS.

**Transferability to ImageNet** We test the transferability by transferring the architecture searched on CIFAR10 to ImageNet. Results in Table 2 show that the SparseNAS architecture learned on CIFAR10 can achieve competitive performance when transferring to ImageNet.

Figure 3: Architectures searched on CIFAR-10 and TinyImageNet.
Table 3: Performance Comparison on TinyImageNet

| Architecture                  | Test Error (%) | Params (M) | Architecture Type |
|-------------------------------|----------------|------------|-------------------|
| DenseNet-BC[16]               | 37.1           | --         | manual            |
| DARTS [27]                   | 46.1           | 2.1        | Single-Path       |
| DARTS+ [23]                  | 28.3           | 3.8        | Single-Path       |
| SparseNAS + HAPG             | 30.1           | 3.8        | Mixed-Path        |
| SparseNAS + AdamHAPG         | 31.9           | 3.1        | Mixed-Path        |

Tiny-ImageNet-200 Performances of searched architectures with HAPG and AdamHAPG is reported in Table 3. The direct search result of DARTS and DARTS+ on TinyImageNet are presented here as a comparison. The result shows that the direct search of DARTS performs badly. This is due to "DARTS Collapse"[23] that DARTS tends to involve excessive skip-connects when training becoming harder. "DARTS Collapse" is caused by the exclusive comparison method[12], which is actually the limitation of Single-Path Architecture Search. Compared to DARTS, our SparseNAS can search much better architectures, because Multi-Path Architecture Search will search for a good combination of paths instead of only the best single path. This shows that Multi-Path Architecture can avoid local minimum of Single-Path Architecture Search. Note that DARTS+ proposed to solve "DARTS Collapse" via early stopping which is an orthogonal contribution to our SparseNAS and similar mechanism can be applied to improve SparseNAS.

In Fig.3, we present architectures searched on CIFAR-10 and TinyImageNet. Particularly, we can get compact reduction cells with only 2 remained intermediate nodes, which proves our advantage on group-level sparsity compared with DSO-NAS [41]. Compared with BayesNAS [44], the total number of paths in normal and reduction cells is fewer as we can achieve better element-level sparsity. In addition, compared to the competing methods, the searched architectures by the proposed SparseNAS show more general properties, such as more diverse path and node structures.

6.2.1 Ablation Study

In Table 4, we compare the performance of conventional Adam algorithm to our proposed AdamHAPG, and we also study the effect of different $\alpha$ in AdamHAPG based architecture search. In Fig.4, we study the effect of the pathwise increasing strategy on $\lambda$, which is increased linearly with a certain step size, to the training stability of search process. As the step size increasing we see a large fluctuation in terms of valid accuracy, while small step sizes lead to much more stable training. Therefore, we enforce a small value like 0.01 or 0.001 to the step size in all our experiments.

Table 4: Comparison between Adam and AdamHAPG and ablation study on $\alpha$

|                  | Test Error (%) | Params (M) |
|------------------|----------------|------------|
| Adam             | 2.93           | 3.30       |
| AdamHAPG($\alpha=0.3$) | 3.30           | 2.67       |
| AdamHAPG($\alpha=0.5$) | 2.69           | 4.20       |
| AdamHAPG($\alpha=0.7$) | 2.79           | 3.98       |

Figure 4: Valid accuracy during search stage with different $\lambda$ steps

7 Conclusions

In this work, we launch Neural Architecture Search to explore in a more general and flexible Mixed-Path Search space using a sparse supernet. Starting from a supernet parameterized by architecture weight factors, we exploit the Sparse Group Lasso regularization on weight factors to automatically search for optimal structures of nodes and paths. To address the challenging optimization problem with non-differentiable sparsity constraint, we propose novel hierarchical proximal algorithms and incorporate them into a bi-level optimization framework. We experimentally show very competitive results and potentials of our derived Mixed-Path architectures on various datasets. We believe that our general Mixed-Path Search modeling will lead the future NAS research to a much broader search space and bring the possibility to derive more flexible and powerful architectures.
Acknowledgement

We would like to thank the AWS Activate team for offering us a round of Cloud Computing Credits used in this work.

8 Broader Impact

Designing neural nets manually is extremely time intensive, and generally requires expensive expertise knowledge that highly limits its use to a smaller community of scientists and engineers. Hence, the research on Neural Architecture Search (NAS) is very valuable, with it allowing machines to automatically discover architectures far more complicated and optimal than what humans may think to try, and these architectures can be optimized for particular goals. However, most traditional NAS methods still require more or less human intervene such as enforcing rigid structure constraints on the final neural architecture. The proposed NAS methodology can be highly expected to reduce such remaining network engineering effort using a more general sparse supernet modeling as well as a promising optimization algorithm. In addition, this fundamental contribution to NAS has a high potential of being applied to a wide range of computer vision and machine learning domains which highly demand good network designs.

Nevertheless, automating the design of neural architectures is still far away from the aim of building fully automated machine learning or artificial general intelligence systems, which also requires automated data selection and loss function search that generally influence the power of neural networks. Accordingly, over-optimizing the design of neural architectures inevitably leads to overfitting the training data and finally reaches a local minimum.

References

[1] F. Alimoglu and E. Alpaydin. Methods of combining multiple classifiers based on different representations for pen-based handwritten digit recognition. In Proceedings of the Fifth Turkish Artificial Intelligence and Artificial Neural Networks Symposium (TAINN 96). Citeseer, 1996.
[2] J. M. Alvarez and M. Salzmann. Learning the number of neurons in deep networks. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, Advances in Neural Information Processing Systems 29, pages 2270–2278. Curran Associates, Inc., 2016.
[3] F. Bach, R. Jenatton, J. Mairal, and G. Obozinski. Optimization with sparsity-inducing penalties. Foundations and Trends® in Machine Learning, 4(1):44–49, 2012.
[4] A. Beck and M. Teboulle. A fast iterative shrinkage-thresholding algorithm for linear inverse problems. SIAM journal on imaging sciences, 2(1):183–202, 2009.
[5] H. Cai, L. Zhu, and S. Han. Proxylessnas: Direct neural architecture search on target task and hardware. arXiv preprint arXiv:1812.00332, 2018.
[6] J. Chang, Y. Guo, G. MENG, S. XIANG, C. Pan, et al. Data: Differentiable architecture approximation. In Advances in Neural Information Processing Systems, pages 874–884, 2019.
[7] W. Chen, X. Gong, X. Liu, Q. Zhang, Y. Li, and Z. Wang. Fasterseg: Searching for faster real-time semantic segmentation. arXiv preprint arXiv:1912.10917, 2019.
[8] X. Chen, L. Xie, J. Wu, and Q. Tian. Progressive darts: Bridging the optimization gap for nas in the wild. arXiv preprint arXiv:1912.10952, 2019.
[9] Y. Chen, G. Meng, Q. Zhang, S. Xiang, C. Huang, L. Mu, and X. Wang. Renas: Reinforced evolutionary neural architecture search. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pages 4787–4796, 2019.
[10] M. Cho, M. Soltani, and C. Hegde. One-shot neural architecture search via compressive sensing. CoRR, abs/1906.02869, 2019.
[11] X. Chu, X. Li, Y. Lu, B. Zhang, and J. Li. Mixpath: A unified approach for one-shot neural architecture search. arXiv preprint arXiv:2001.05887, 2020.
[12] X. Chu, T. Zhou, B. Zhang, and J. Li. Fair darts: Eliminating unfair advantages in differentiable architecture search. arXiv preprint arXiv:1911.12126, 2019.
[13] J. Deng, W. Dong, R. Socher, L. Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In 2009 IEEE Conference on Computer Vision and Pattern Recognition, pages 248–255, 2009.
14] X. Gong, S. Chang, Y. Jiang, and Z. Wang. Autogan: Neural architecture search for generative adversarial networks. In *Proceedings of the IEEE International Conference on Computer Vision*, pages 3224–3234, 2019.

15] A. G. Howard, M. Zhu, B. Chen, D. Kalenichenko, W. Wang, T. Weyand, M. Andreetto, and H. Adam. Mobilenets: Efficient convolutional neural networks for mobile vision applications. *CoRR*, abs/1704.04861, 2017.

16] G. Huang, Z. Liu, and K. Q. Weinberger. Densely connected convolutional networks. *CoRR*, abs/1608.06993, 2016.

17] Z. Huang and N. Wang. Data-driven sparse structure selection for deep neural networks. *CoRR*, abs/1707.01213, 2017.

18] Y. Ida, Y. Fujiwara, and H. Kashima. Fast sparse group lasso. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems 32*, pages 1702–1710. Curran Associates, Inc., 2019.

19] D. P. Kingma and J. Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

20] A. Krizhevsky. Learning multiple layers of features from tiny images. *University of Toronto, 05 2012*.

21] G. Li, G. Qian, I. C. Delgadillo, M. Müller, A. Thabet, and B. Ghanem. Sgas: Sequential greedy architecture search. *arXiv preprint arXiv:1912.00195*, 2019.

22] Y. Li, S. Gu, C. Mayer, L. Van Gool, and R. Timofte. Group sparsity: The hinge between filter pruning and decomposition for network compression. *arXiv preprint arXiv:2003.08935*, 2020.

23] H. Liang, S. Zhang, J. Sun, X. He, W. Huang, K. Zhuang, and Z. Li. Darts+: Improved differentiable architecture search with early stopping. *arXiv preprint arXiv:1909.06035*, 2019.

24] C. Liu, L.-C. Chen, F. Schroff, H. Adam, W. Hua, A. L. Yuille, and L. Fei-Fei. Auto-deeplab: Hierarchical neural architecture search for semantic image segmentation. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 82–92, 2019.

25] C. Liu, B. Zoph, M. Neumann, J. Shlens, W. Hua, L.-J. Li, L. Fei-Fei, A. Yuille, J. Huang, and K. Murphy. Progressive neural architecture search. In *Proceedings of the European Conference on Computer Vision (ECCV)*, pages 19–34, 2018.

26] H. Liu, K. Simonyan, O. Vinyals, C. Fernando, and K. Kavukcuoglu. Hierarchical representations for efficient architecture search. *arXiv preprint arXiv:1806.09055*, 2018.

27] H. Liu, K. Simonyan, and Y. Yang. DARTS: Differentiable architecture search. *arXiv preprint arXiv:1711.04436*, 2017.

28] Z. Liu, J. Li, Z. Shen, G. Huang, S. Yan, and C. Zhang. Learning efficient convolutional networks through network slimming. In *Proceedings of the IEEE International Conference on Computer Vision*, pages 2736–2744, 2017.

29] R. Luo, F. Tian, T. Qin, E. Chen, and T.-Y. Liu. Neural architecture optimization. In *Advances in neural information processing systems*, pages 7816–7827, 2018.

30] E. Real, A. Aggarwal, Y. Huang, and Q. V. Le. Regularized evolution for image classifier architecture search. In *Proceedings of the aaai conference on artificial intelligence*, volume 33, pages 4780–4789, 2019.

31] S. Scardapane, D. Comminiello, A. Hussain, and A. Uncini. Group sparse regularization for deep neural networks. *Neurocomputing*, 241:81–89, 2017.

32] N. Simon, J. Friedman, T. Hastie, and R. Tibshirani. A sparse-group lasso. *Journal of Computational and Graphical Statistics*, 22(2):231–245, 2013.

33] N. Simon, J. Friedman, T. Hastie, and R. Tibshirani. A sparse-group lasso. *Journal of computational and graphical statistics*, 22(2):231–245, 2013.

34] C. Szegedy, W. Liu, Y. Jia, P. Sermanet, S. Reed, D. Anguelov, D. Erhan, V. Vanhoucke, and A. Rabinovich. Going deeper with convolutions. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 1–9, 2015.

35] W. Wen, C. Wu, Y. Wang, Y. Chen, and H. Li. Learning structured sparsity in deep neural networks. In *Advances in neural information processing systems*, pages 2074–2082, 2016.

36] B. Wu, X. Dai, P. Zhang, Y. Wang, F. Sun, Y. Wu, Y. Tian, P. Vajda, Y. Jia, and K. Keutzer. Fbnet: Hardware-aware efficient convnet design via differentiable neural architecture search. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 10734–10742, 2019.

37] S. Xie, R. Girshick, P. Dollár, Z. Tu, and K. He. Aggregated residual transformations for deep neural networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 1492–1500, 2017.

38] S. Xie, H. Zheng, C. Liu, and L. Lin. Snas: stochastic neural architecture search. *arXiv preprint arXiv:1812.09926*, 2018.
Appendix

A Experimental Details

A.1 Network Pruning

A.1.1 Architecture Search

For the four implemented algorithms, SGD, Adam, HAPG, AdamHAPG in the network pruning experiment, we train for 500 epochs with batch size 256 in search stage. For SGD, we employ momentum SGD with momentum 0.9 and initiate the learning rate as 0.025 with an annealing cosine decay schedule. For Adam, we initiate the learning rate as $3 \times 10^{-4}$ and set momentum (0.5, 0.999). For HAPG, we initiate the learning rate as 0.05 with an cosine annealing decay schedule. For AdamHAPG, the initial learning rate is set to be $3 \times 10^{-4}$ and as for the Adam gradient update, we employ momentum (0.5, 0.999).

A.1.2 Architecture Evaluation

We evaluate the final sparse network after the architecture search stage. As SGD and Adam cannot directly derive a sparse network, a hard threshold is necessary and here we set the threshold as 0.001, i.e., discard the inner connections with weights smaller than 0.001 and discard neurons with all outgoing weights below 0.001. For HAPG and AdamHAPG, we simply zero out connections and neurons with zero weights. The final architecture is trained with Adam for 3000 epochs. The initiate learning rate is set to be $3 \times 10^{-4}$ and use momentum (0.5, 0.999).

A.2 Neural Architecture Search

A.2.1 Architecture Search

In the architecture search stage, we optimize the supernet for 50 epochs with batch size 64. The supernet is a stack of 8 basic cells and each cell has 7 nodes with 2 inputs and one single output node. The channel number is set to be 16. To optimize the network parameters $w$, we employ SGD momentum with momentum 0.9, weight decay $3 \times 10^{-4}$ and initiate the learning rate as 0.025 (an annealing cosine decay schedule is applied). To optimize the architecture weight factors $A$, we employ proposed HAPG and AdamHAPG. For HAPG, we initiate the learning rate as 0.025 with an annealing cosine decay schedule. For AdamHAPG, the initial learning rate is $3 \times 10^{-4}$ and for the Adam update step, the momentum is (0.5, 0.999). The search space is similar as DARTS without zero, which includes skip-connect, max-pool-3×3, avg-pool-3×3, sep-conv-3×3, sep-conv-5×5, dil-conv-3×3, dil-conv-5×5.
Table 5: Transferability Comparison on ImageNet in the Mobile Setting. * represents that the results are searched directly on ImageNet; † represents that the results are search on TinyImageNet; Otherwise, they are searched on CIFAR10.

| Architecture | Test Error (%) | Params (M) | Architecture Type |
|--------------|----------------|------------|-------------------|
| Inception-v1 [34] | 30.20/10.1 | 6.6 | manual |
| MobileNet [15] | 29.40/10.5 | 4.2 | manual |
| DARTS[27] | 26.70/8.7 | 4.7 | Single-Path |
| P-DARTS[8] | 24.40/7.4 | 4.9 | Single-Path |
| MixPath*[11] | 22.80/6.5 | 5.1 | Multi-Path |
| DSO-NAS[41] | 26.20/8.6 | 4.7 | Mixed-Path |
| BayesNAS[44] | 26.50/8.9 | 3.9 | Mixed-Path |
| SparseNAS | 24.67/7.6 | 5.7 | Mixed-Path |
| SparseNAS† | 25.25/8.0 | 5.2 | Mixed-Path |

Searching in Small Search Space Mixed-Path architecture search without any constraints explores in a huge search space (1 × 10^57). Thus we design a small search space comparable with DARTS to show Mixed-Path architecture’s advantage and potential. We shrink the search space with only sep-conv-3×3, skip-connect for normal cell and skip-connect, max-pool-3×3 for reduce cell. The search space scale with Mix-Path Architecture is approximately 1 × 10^17, while DARTS is approximately 1 × 10^18. Other settings are similar as before.

A.2.2 Architecture Evaluation

Evaluation on CIFAR10/100 The architecture searched on CIFAR10 is evaluated on CIFAR10 and transferred to CIFAR100. As CIFAR100 is highly related to CIFAR10, we do not do direct search on CIFAR100 redundantly. Following DARTS, we stack the extracted cells for 20 times and use 36 initial channels for evaluation network. As the architecture topology from Mix-Path search is relatively complex, we train the network for 1200 epochs to ensure convergence. We also add cutout, path dropout with probability 0.2 and auxiliary towers with weight 0.4. Meanwhile, the architecture from small search space is trained with the same setting as DARTS.

Transferability to ImageNet For ImageNet mobile setting, the size of input images is 224×224. The cell is stacked for 14 times an trained for 250 epochs with batch size 512, weight decay 3 × 10^-5, SGD optimizer and linear learning decay with initial learning rate to be 0.4.

Tiny-ImageNet-200 Similar as CIFAR10/100, the network uses 20 cells and 36 channels. An additional 3×3 convolution layer with stride 2 is inserted in the first layer. Other experimental settings are the same as CIFAR10/100.

B Transferability to Imagenet

In addition to the transfer results from CIFAR10 to ImageNet, we transfer the architecture searched on TinyImageNet to ImageNet and the results are presented in Table 5. The results show that the searched architecture by our SparseNAS on TinyImageNet is comparable with the one searched on CIFAR10, which shows that our SparseNAS is capable to search for architectures with good transferability on various datasets.

C Visualization of Searched Architectures

We visualize all the architectures searched on CIFAR-10 in Figure 5 and architectures searched on TinyImageNet in Figure 6. Both HAPG and AdamHAPG are able to generate more general structure with flexible paths and nodes. In particular, all the resulting reduction cells are more compact with less paths and nodes.
Figure 5: Architectures searched on CIFAR-10

Figure 6: Architectures searched on TinyImageNet

References

[1] Zoph, B.; Le, Q. V. Neural architecture search with reinforcement learning. arXiv preprint arXiv:1611.01578 2016,

[2] Liu, H.; Simonyan, K.; Vinyals, O.; Fernando, C.; Kavukcuoglu, K. Hierarchical representations for efficient architecture search. arXiv preprint arXiv:1711.00436 2017,

[3] Zoph, B.; Vasudevan, V.; Shlens, J.; Le, Q. V. Learning transferable architectures for scalable image recognition. Proceedings of the IEEE conference on computer vision and pattern recognition. 2018; pp 8697–8710.

[4] Liu, H.; Simonyan, K.; Yang, Y. DARTS: Differentiable architecture search. arXiv preprint arXiv:1806.09055 2018,

[5] Real, E.; Aggarwal, A.; Huang, Y.; Le, Q. V. Regularized evolution for image classifier architecture search. Proceedings of the aaai conference on artificial intelligence. 2019; pp 4780–4789.