Self-supervised Neural Architecture Search

Sapir Kaplan and Raja Giryes
School of Electrical Engineering
Tel Aviv University
raja@tauex.tau.ac.il

Abstract

Neural Architecture Search (NAS) has been used recently to achieve improved performance in various tasks and most prominently in image classification. Yet, current search strategies rely on large labeled datasets, which limit their usage in the case where only a smaller fraction of the data is annotated. Self-supervised learning has shown great promise in training neural networks using unlabeled data. In this work, we propose a self-supervised neural architecture search (SSNAS) that allows finding novel network models without the need for labeled data. We show that such a search leads to comparable results to supervised training with a “fully labeled” NAS and that it can improve the performance of self-supervised learning. Moreover, we demonstrate the advantage of the proposed approach when the number of labels in the search is relatively small.

1 Introduction

Recently there has been an increasing interest in Neural Architecture Search (NAS). NAS algorithms emerge as a powerful platform for discovering superior network architectures, which may save time and effort of human-experts. The discovered architectures have achieved state-of-the-art results in several tasks such as image classification [1, 2] and object detection [3].

The existing body of research on NAS investigated several common search strategies. Reinforcement learning [4] and evolutionary algorithms [5, 6] were proven to be successful but required many computational resources. Various recent methods managed to reduce search time significantly. For example, Liu et al. [7] suggested relaxing the search space to be continuous. This allowed them to perform a differentiable architecture search (DARTS), which led to novel network models and required reasonable resources (few days using 1-4 GPUs).

NAS methods learn from labeled data. During the search process, various architectures are considered and their value is estimated based on their performance on annotated examples. However, acquiring large amounts of human-annotated data is expensive and time-consuming, while unlabeled data is much more accessible. As current NAS techniques depend on annotations availability, their performance deteriorates when the number of annotations per each class becomes small. This remains an open problem for NAS, where research till now has focused on the supervised learning approach.

The dependency on labeled data is not unique only to NAS but is a common problem in deep learning. Large-scale annotated datasets play a critical role in the remarkable success of many deep neural networks, leading to state-of-the-art results in various computer vision tasks. Considering how expensive it is to acquire such datasets, a growing body of research is focused on relieving the need for such extensive annotation effort. One promising lead in this direction is self-supervised learning (SSL) [8, 9, 10]. Self-supervised methods learn visual features from unlabeled data. The unlabeled data is used to automatically produce pseudo labels for a pretext task. In the course of training to solve the pretext task, the network learns visual features that can be transferred to solving other tasks with little to no labeled data. Contrastive SSL is a subclass of SSL that has recently gained...
Figure 1: **The SSNAS framework.** We perform network architecture search in an unsupervised manner (with no data labels) by using a contrastive loss that enforces similarity between two different augmentations of the same input image. Both augmentations pass through the same network (i.e., the weights are shared).

attention thanks to its promising results [11][12][13][14][15]. This family of techniques contrasts positive samples and negative samples to learn visual representations.

**Contribution.** Inspired by the success of SSL for learning good visual representations, we propose to apply self-supervision in NAS to rectify its limitation with respect to the availability of data annotations. We propose a Self-Supervised Neural Architecture Search (SSNAS), which unlike conventional NAS techniques, can find novel architectures without relying on data annotations. Instead of using self-supervision to learn visual representations, we employ it to learn the architecture of deep networks (see Figure 1).

We apply our new strategy with the popular DARTS [7] method. We adopt their differentiable search, which allows using gradient-based optimization, but replace their supervised learning objective with a contrastive loss that requires no labels to guide the search. In particular, we adopt the method used in the SimCLR framework [11]. This approach for learning visual representations has recently achieved impressive performance in image classification. We adapt their approach to the architecture search process. We perform a composition of transformations on the inputs, which generates augmented images and look for the model that maximizes the similarity between the representations of the augmented images that originate from the same input image. As the focus of this work is on efficient search, we limit the used batch sizes to be the ones that can fit a conventional GPU memory. This allows SSNAS to efficiently learn novel network models without using any labeled data.

We demonstrate that our self-supervised approach for NAS achieves results comparable to the ones of its equivalent supervised approach. Moreover, we show that SSNAS not only achieves the same results as supervised NAS, but it also succeeds in some scenarios where the supervised method struggles. Specifically, SSNAS can learn good architectures from data with a small number of annotated examples available for each class. We also demonstrate the potential of using NAS to improve unsupervised learning. We show some examples where SSL applied with the learned architectures generates visual representations that lead to improved performance. Thus, this work shows that SSL can both improve NAS and be improved by it.
2 Related work

Neural architecture search. The first methods to perform neural architecture search focused on using reinforcement learning [4] and evolutionary (genetic) algorithms [5, 6]. They have shown that the architecture found using these techniques outperform the performance achieved by manually designed models. The disadvantage of these approaches is their very long search time and the need for a significant amount of resources.

To overcome the computational issue, efficient search techniques have been proposed. These include the effective NAS (ENAS) [16] and the differentiable architecture search (DARTS) [7]. The first reduce the computational load of RL models using a graph structure and the second model the search in a differentiable manner, which makes it computationally efficient. These approaches have been further extended to make the search more efficient [17, 18, 19, 20, 21, 22, 23] and also for applying it to applications beyond classification such as semantic segmentation [24], medical image segmentation [25, 26], object detection [27], image generation [28], few-shot learning [29], etc.

One of the disadvantages of the search methods is that they require labeled data to perform the search. Moreover, when the number of training examples per class in a given dataset is low, the search becomes less stable. For example, while DARTS gets very good network architectures on CIFAR-10 [30] that has 5000 labeled examples per class, its performance degrades significantly on CIFAR-100 [30], where each class contains only 500 labeled examples per class. Follow-up works [19, 20] have added a regularization on the searched operations to mitigate these issues. Yet, an important question is whether such regularizations that require prior knowledge on the target network structure are needed.

In this work, we show that one may perform a search on the data without the labels at all, which leads to a stable search using even vanilla DARTS. Moreover, it allows performing the search on datasets with no (or only a few) labels where none of the above methods is applicable.

Self-supervised learning. A considerable amount of literature was published on self-supervised representation learning. These studies suggested various pretext tasks where pseudo labels generated from unlabeled datasets drive networks to learn visual features. There is a wide choice of such pretext tasks available in the literature: predicting patch position [8], image colorization [9], jigsaw puzzles [10], image inpainting [31], predicting image rotations [32], etc. Using this approach, researchers achieved good results. However, the generality of the representations produced is arguably limited due to the specific nature of the pretext tasks.

Recent attention was given to the contrastive self-supervised learning [11, 12, 13, 14, 15]. Methods that use this concept such as SimCLR [11] and MoCo [12] attained promising results, narrowing significantly the gap between supervised and unsupervised learning. SimCLR [11] employed a composition of data augmentations on input images to create different views of the same image and used a nonlinear head on the representation before applying a contrastive loss. MoCo [12] maintained a dynamic dictionary and aimed at maximizing the similarity between an encoded query and keys encoded by a slowly progressing momentum encoder. The follow-up work, MoCo v2 [13] adopted a few techniques from SimCLR to further improve MoCo performance.

3 Method

Our SSNAS framework aims at finding effective models without using data annotations. Instead, it learns by maximizing the similarity between projected representations of different views originating from the same input image. We focus on the case of limited resources and opt for approaches we can carry out using a single GPU.

Our approach is inspired by the following key observation: Virtually, all currently used networks overfit the training data, i.e., if we compare the randomly sampled networks to the found ones, all of them attain close to zero training error. Therefore, the difference between them is their generalization ability. In other words, the search goal is to find the training architecture that inherently generalizes best the data.

Given the above, an important question is whether we can find networks that generalize well without using the labels? To do so, we first revisit the NAS problem and present it from the perspective of learning to generalize well on the training data. Then we discuss how one may improve generalization
without access to the labels. Namely, we rely on recent theoretical findings that show that networks with a large margin exhibit good generalization abilities \[33, 34, 35, 36, 37\].

With this perspective in mind, we suggest using a recent self-supervised technique, SimCLR, which uses the contrastive loss that increases the network margin in an unsupervised way, to perform an unsupervised architecture search (we demonstrate our approach on the DARTS strategy). Specifically, we train the network on one part of the data to increase the margin between examples and select the network architecture that succeeds to maintain the largest distance between samples that were not present during training (i.e., the one that can achieve the largest margin). We start by presenting our general framework and then briefly describe the used SimCLR and DARTS approaches.

### 3.1 Margin based search

In essence, any architecture search technique splits the data into two parts, the train set \(T_T\) and the validation set \(T_V\), and then tries to find the best architecture \(f_W\) (with a set of weights \(W\)) from a certain search space \(A\) that leads to the best performance on the validation set, i.e., it aims at solving an optimization problem of the form

\[
\min_{f_W \in A} E(f_W^*, T_V) \quad \text{s.t.} \quad W^* = \arg\min_W E(f_W, T_T),
\]

where \(E(f_W, T)\) is the error of the network \(f_W\) on the dataset \(T\). Let us now assume that all the networks in the search space are capable of attaining an error close to zero, i.e.,

\[
\min_W E(f_W, T_T) \leq \epsilon, \quad \forall f_W \in A.
\]

Under this assumption, we may rewrite Eq. (1) as

\[
\min_{f_W \in A} E(f_W^*, T_V) - E(f_W^*, T_T) \quad \text{s.t.} \quad W^* = \arg\min_W E(f_W, T_T).
\]

The term \(E(f_W^*, T_V) - E(f_W^*, T_T)\) is known as the generalization error of the network (to be precise, we need to replace \(E(f_W^*, T_V)\) with the expected error over all the data; yet the validation error is often considered to be a good proxy of the latter). Clearly, the error in the optimal architecture found by solving Eq. (3) is the same as the one found by solving Eq. (1) up to an \(\epsilon\) difference.

The above discussion suggests that instead of minimizing the error in the search (as in Eq. (1)), one may aim at finding the model that is capable of attaining the smallest generalization error (as in Eq. (3)). Performing a search using the latter still requires having the data labels. Yet, in the literature, various measures have been developed to upper bound the generalization error of the network \[38, 39\].

In this work, we focus on the margin-based approach that relates the generalization error of the network to the margin of the network \[33, 34, 35, 36, 37\]. These works show that increasing the margin of the network, i.e., the distance from the training examples to the decision boundary of the network, improves the network’s generalization error. Moreover, it is shown that if we make a network invariant to different augmentations, its generalization error improves \[40\].

Therefore, we suggest replacing the labeled based search with an unsupervised search that maximizes the margin. While there are many possible directions to perform this, we focus on a self-supervised learning-based approach that optimizes the embedding space.

### 3.2 The Contrastive Loss for Self-supervised Search

To search without using labels, we adopt the SSL approach of SimCLR \[11\]. First, a composition of random data augmentations (e.g. crop and resize, horizontal flip, color distortion and gaussian blur) is applied to input images. The augmentations of the same input are considered to be a positive pair and the augmentations of different inputs are considered to be negative pairs. The distance between views of positive pairs is minimized while the distance between negative samples is maximized.

Consider such an optimization from a margin perspective. If each input image is a class, then the optimization aims at finding the feature space with the largest margin between these classes. A network capable of finding a feature space with a large margin in this case, is also expected to find a feature space with a large margin when the classes correspond to groups of multiple input examples. (In that case, we are only concerned with the margin between the classes, which is an easier task). This provides us with a proxy loss for NAS when not enough labels are available for the search.
In view of the above, we expect that applying NAS with a SimCLR objective will lead to finding network architectures that have good generalization properties, which is exactly our goal in the optimization in Eq. (3). While SimCLR uses a fixed ResNet \([41]\) to learn effective visual representation, we use our dynamic network of stacked cells with mixed operations (following the DARTS approach) to learn an effective network architecture. This choice enables us to increase the network margin by contrasting positive pairs and negative pairs generated on the fly.

Before we turn to show empirically that indeed, using this loss in NAS leads to comparable results to the supervised search, we briefly describe the DARTS approach and the SimCLR strategy in more detail. A reader that is familiar with these methods may skip directly to Section 4.

### 3.3 Differential Architecture Search

We perform neural architecture search by adapting the framework of DARTS \([7]\). We search for a cell to be stacked to a deep network. Searching for a cell that serves as a building block for the final architecture is an efficient approach yet it comes at the expense of optimality.

A cell is represented by a directed acyclic graph (DAG) of \(N\) nodes \(\{x_i\}_{i=0}^{N-1}\). Node \(x_i\) represents a feature map and edge \((i, j)\) represents an operation \(o_{(i,j)}\) performed on \(x_i\). Cell input nodes are the outputs of two previous cells. Intermediate nodes are obtained by summing the operations performed on previous nodes: \(x_j = \sum_{i<j} o_{(i,j)}x_i\). Cell output is a concatenation of all intermediate nodes.

During the search, operations are selected from the set \(O\), which contains the possible operations (e.g. convolution, pooling, identity and zero). To relax the search space, instead of having a specific operation \(o_{i,j}\) applied to each node \(x_i\), a mixture of operations is applied, i.e., we have a weighted sum of all possible operations: The candidate operations are weighted by the \(\alpha_{(i,j)}\) vectors. A softmax is applied over all the weights in \(\alpha_{(i,j)}\) to emphasize the ones with the larger weights. To obtain a discrete architecture once search is concluded, we select the most dominant operation by applying argmax on the \(\alpha_{(i,j)}\) vectors. The set \(\alpha = \{\alpha_{(i,j)}\}\) (after the pruning) encodes the architecture. To form the final network, the stacked cells are preceded by a convolutional layer and followed by a global pooling and a linear layer (with softmax at the end).

The architecture \(\alpha\) and the network’s weights are learned jointly via solving a bilevel optimization problem. To solve it, the architecture gradient is computed via approximation of the weights that minimize the training loss (instead of training the network fully). According to a second-order approximation, those weights are computed by performing a single train step. The first-order approximation simply uses the current weights. Using this approximation rather than the second-order one speeds up the search, yet it comes at the cost of reduced performance.

### 3.4 The SimCLR approach

In SimCLR each input image \(x\), is augmented twice, forming a positive pair \(\tilde{x}_i\) and \(\tilde{x}_j\). Then, the augmented views are passed through our network of stacked cells (as in the DARTS model). Denoting the output of the network final pooling layer by \(h_i\), an MLP \(g(\cdot)\) is used to project it to a latent space, obtaining \(z_i = g(h_i)\). As SimCLR demonstrated, this mapping is effective as presumably, it allows \(h_i\) to keep all the information necessary for classification, while \(z_i\) can discard some of it to predict the agreement between pairs of views more accurately.

In a batch of \(N\) input images, there are \(2N\) augmented images. Among them, each pair of augmented views, namely \(\tilde{x}_i\) and \(\tilde{x}_j\), form a positive pair, while the other pairs serve as negative examples. For each positive pair, we use the normalized temperature-scaled cross entropy loss \([11]\):

\[
\ell_{i,j} = -\log \frac{\exp\left(\frac{\text{sim}(z_i, z_j)}{\tau}\right)}{\sum_{k=1}^{2N} 1[z_k] \exp\left(\frac{\text{sim}(z_i, z_k)}{\tau}\right)},
\]

where \(\text{sim}(z_i, z_j) = \frac{z_i^\top z_j}{\|z_i\|\|z_j\|}\) denotes the cosine similarity, \(1\) is an indicator function and \(\tau\) is a temperature hyperparameter.
4 Experiments

We turn to test our SSNAS approach and conduct a self-supervised architecture search to identify novel architectures without using labeled data. To evaluate the learned cells, we measure the performance of the found architectures using labeled data. To further examine our approach, we experiment with self-supervised pretraining \(^1\) in the case of limited resources and evaluate the learned representations for classification with limited annotations. We show that using the learned architectures with SSL can improve the learned representations.

Datasets. We conduct most of our search experiments on CIFAR-10 [30]. In this case, we show that search with and without labels lead virtually to the same performance. To evaluate cell transferability, we train learned cells on ImageNet [42]. Then, we turn to other datasets where the number of available labels per class is relatively small. These include CIFAR-100 [30], where the vanilla DARTS [7] struggles, and STL-10 [43], where the number of labels is significantly small and thus applying supervised NAS techniques is very challenging.

4.1 Implementation details

We describe now the setup we use for the architecture search with the SSL loss, both in the training and the evaluation phases. We also detail the SSL pretraining with the learned architectures.

Architecture search. We use the same setup that was detailed in DARTS [7]. We learn a normal cell and a reduction cell, each consisting of 7 nodes. The candidate operations include separable convolutions and dilated separable convolutions (3x3, 5x5), average pooling (3x3), max pooling (3x3), zero, and identity. To obtain the final cell after the search concludes, we keep for each node the two strongest operations (among all the operations from the predecessor nodes). By stacking the cells, we form a deep network. As search results might be sensitive to initialization, we run the search four times with different random seeds.

In order to generalize well on the training data, we keep the procedural choice of separating the original training set into two separate sets, where one is used to learn the network weights while the other pushes towards a network structure with an increased margin.

To solve the optimization problem, we use the first-order approximation of the gradient which requires fewer resources (even though it comes at the cost of reduced performance, we were still able to use it to get performance comparable to DARTS).

Though SSL frameworks achieve state-of-the-art results by using many computation resources (namely SimCLR uses large batch sizes up to 8192 and up to 128 cores of TPUs), we focus on the case of limited resources: We use small batch sizes and work with models that fit in a single GPU.

Architecture evaluation. To select which model to evaluate, we employ the following model selection strategy as in [7]: We train each network for a small number of epochs (100) and pick the best model based on its performance on a validation set. To evaluate the final architecture, we train the network from scratch and test it on a test set. The network used for model selection and training is larger than the one used for search (8 cells for search and 20 cells for training), and also the number of input channels is higher (16 channels for search and 36 channels for training).

Self-supervised pretraining. For pretraining, we adapt the procedure used in SimCLR [11]. We use our learned architecture as the base network, and add a nonlinear head on top of it (namely an MLP with two layers and a ReLU nonlinearity). The representations are mapped to 128-dimensional projections. The composition of random augmentations includes random crop and resize, random horizontal flip, color distortion, and Gaussian blur. As we investigate the case of limited resources, we use small batch sizes of 32 and 64 on a single GPU (unlike the original SimCLR [11] framework that experimented with batches of size up to 8192 and used up to 128 TPU cores). The same settings are used also in SSNAS (to enforce the contrastive loss and perform the search without annotations).

Evaluation of the self-supervised learned representations. We evaluate the learned representations using the common linear evaluation protocol [9, 11, 15]. We freeze the pretrained network and add a linear classifier on top of it, and train it on the entire train set.

\(^1\) Here and elsewhere in the paper pretraining refers to unsupervised pretraining by SSL.
Table 1: Image classification test error on CIFAR-10

| Architecture          | Search Type | Test Error (%) |
|-----------------------|-------------|----------------|
| Random sampling       | random      | 3.29           |
| DARTS [7] (first order) | supervised | 3.00           |
| DARTS [7] (second order) | supervised | 2.62           |
| SSNAS (first order)   | self-supervised | 2.61         |

Table 2: Image classification test errors on ImageNet

| Architecture          | Search Type   | Test Error (%) |
|-----------------------|---------------|----------------|
|                      |               | top-1 top-5    |
| DARTS [7] (second order) | supervised | 28.92 10.24  |
| SSNAS (first order)   | self-supervised | 27.75 9.55  |

We also evaluate the learned representation in a semi-supervised setting. We sample 10% of the labels in a given labeled dataset and fine-tune the entire pretrained network on the labeled data. We conclude with testing the fine-tuned model on the test set. For datasets that are already suitable for semi-supervised learning (e.g., STL), we use the few provided examples (instead of taking a fraction of the annotations). These experiments show the potential of the learned architecture to contribute to visual representation learning with SSL.

4.2 Learning network architectures from unlabeled data

Comparisons to the fully annotated case. We used our SSNAS framework to search for novel architectures on CIFAR-10 without using any annotations. For model selection, we ran a short supervised train (100 epochs) for each of the learned architectures and measured its performance on the validation set. We then performed a full supervised train (650 epochs) on the selected model and tested it on the test set.

Table 1 compares our results to the baseline (DARTS) that requires data annotations. Notice that our search, which uses only a first-order approximation, is comparable to the results of DARTS with the second-order approximation, which is more computationally demanding in the search stage, and outperforms both the first order DARTS and the random sampling. Remarkably, this is obtained without using any labels during the search.

We investigated cell transferability by evaluating the learned model on ImageNet [42]. We adjusted the model to have 14 cells and 48 input channels. We trained the network from scratch for 250 epochs and tested its performance on the test set. We used the same hyperparameters as in DARTS [7] except for a bigger batch size used to speed up the training. The same settings were used to evaluate our framework and DARTS. Table 2 shows SSNAS results for cell transferability against the results of DARTS. These results confirm that SSNAS matches the performance of the supervised approach also when transferring the architecture.

Comparisons to scarce labels case. We also employed SSNAS to search for architectures on CIFAR-100 (following the same procedure described for CIFAR-10). Table 3 shows comparisons between SSNAS results and the results of the baseline. In this case, we show that our method succeeds while the vanilla DARTS struggles, without adding regularization or employing specific techniques to prevent DARTS collapse. We also show that SSNAS outperforms random sampling as well. This experiment demonstrates the advantage of performing architecture search with no labels when the number of labeled examples per class is relatively small.

4.3 Self-supervised learning using searched models

To investigate the potential of using NAS to improve unsupervised learning, we used the architectures we found for CIFAR-10 as the base network for learning visual representations from CIFAR-10 using SSL in the case of limited annotations. We carried out the model selection by running short pretraining on each of the searched architectures and then selected the best performing network based on the
Table 3: Image classification accuracies on CIFAR-100

| Architecture          | Search Type     | Test Accuracy (%) |
|-----------------------|-----------------|-------------------|
| DARTS \[7\] (first order) | supervised     | 64.46             |
| Random sampling       | random          | 82.61             |
| SSNAS (first order)   | self-supervised | **83.36**         |

Table 4: Learning visual representations from CIFAR-10 (limited-resources scenario)

| Architecture | Batch Size | Linear Evaluation (%) | Semi-supervised (%) |
|--------------|------------|-----------------------|---------------------|
| ResNet-18    | 32         | 87.63                 | 88.85               |
| Random sampling | 32       | 83.48                 | 88.39               |
| SSNAS (first order) | 32     | **88.78**             | **89.45**           |
| ResNet-18    | 64         | 90.53                 | 90.17               |
| Random sampling | 64       | 88.13                 | 90.03               |
| SSNAS (first order) | 64     | **90.87**             | **90.94**           |

model’s contrastive loss on the validation set (without using any annotations). We then pretrained the selected model with a relatively small batch size (32 or 64) as we consider the limited-resources scenario. To evaluate our results, we applied SSL also with randomly selected architectures and with ResNet-18. We compare to ResNet-18 as this is the architecture employed in \[11\] for CIFAR-10. For evaluation, we used the common linear evaluation protocol and the semi-supervised settings.

Table 4 presents our results and compare them to the randomly selected architectures and SimCLR’s base network (ResNet-18). Notice that the learned architecture attains better performance for the batch sizes that are considered compared to both the randomly selected architecture and the ResNet-18 model. This shows the potential of combining SSL with NAS to learn improved visual representations.

To assess the applicability of our framework on datasets that are suitable for semi-supervised learning with only a few labels available, we experimented on STL-10 \[43\]. As the number of annotations is relatively small (500 labeled training examples per class), we cannot apply supervised methods for the search. Instead, we used SSNAS to search for a compact architecture (with 5 cells) that served as the base network for pretraining. In the next step, we used the labeled examples in the training set (5000 training images) to finetune the network. We repeated this procedure several times, with the following changes: (i) using a random architecture instead of the learned one; and (ii) training from scratch (initializing the architecture with random weights) rather than using the weights of the pretrained model. For comparison, we also performed pretraining with ResNet-18 \[41\] as the base model using the same settings. Results of this experiment are presented in Table 5. Fine-tuning the pretrained model learned by SSNAS outperforms fine-tuning the original ResNet-18 model, fine-tuning a random model or using the learned model without the learned weights. This experiment demonstrates the advantage of pretraining with a learned architecture on datasets that are suitable for semi-supervised learning and confirms the potential of NAS to improve SSL.

Table 5: Learning visual representations from STL-10 (semi-supervised setting)

| Architecture          | Fine-tune       | Test Accuracy (%) |
|-----------------------|-----------------|-------------------|
| Random sampling       | pretrained model | 84.55             |
| ResNet-18             | pretrained model | 86.13             |
| SSNAS (first order)   | random weights  | 67.00             |
| SSNAS (first order)   | pretrained model | **86.70**         |
4.4 The train set and the validation set of SSNAS

During the search, we split the data into two parts, a train set used to learn the network weights, and a validation set used to learn the architecture parameter $\alpha$. An interesting question is whether to perform such a split or to use the same set (containing all the samples) for both learning the network’s weights and learning $\alpha$. While for supervised search the first is practiced, we wanted to verify that this is also the preferred choice for our SSL search. Our experiments have shown that indeed using separate sets leads to improved performance compared to using the same set (with twice as many examples): We observe a difference in performance on the test set of 0.63% in favor of splitting the data.

5 Conclusion

In this paper, we present a framework for self-supervised neural architecture search. This study set out to determine whether architecture search can be carried out without using labeled data. Our research has confirmed that indeed it is possible: Our framework matched the performance of equivalent supervised methods without using annotations at all. We have also identified that the learned architectures can be used as the base network in SSL frameworks and improve their performance. In particular, we have shown this advantage for datasets with few labels, i.e., using SSL in the limited annotations scenario. Our findings demonstrate that SSL and NAS can be put in a symbiosis where both benefit from each other.

The focus of this work is exploring the search and training with limited resources. A natural progression of this work is to expand the experiments on SSL to larger models, datasets, and batch sizes. One may also experiment with other recent learning methods such as self-training with noisy student [44]. We believe (although we do not have the resources to check that) that the same advantage will be demonstrated in these cases. Notwithstanding these limitations, the results established in this work already demonstrate the great advantage of using SSL and NAS together.

Another possible follow-up research direction is using an architecture search to learn better augmentations to be used with the self-supervised learning techniques. This can be done for example by extending methods such as auto-augment that searches for the optimal augmentations for a given supervised task [45, 46]. While [11] reported that using the current augmentations found by auto-augment does not improve the learned representations in their method, we believe that by combining the two such that the learned augmentations are designed specifically for the SSL task, the learned visual representations can be improved.

Broader Impact

As SSL relieves the need for expensive and time-consuming annotation efforts, works in this field, ours included, contribute to democratizing AI by enabling any person, researcher or organization to enjoy the benefits of deep learning on their data regardless of their ability to afford and carry out annotation of large scale datasets. NAS also contributes to the same cause: While previously only a select few were able to manually design effective models, NAS automated this process and made it easier to find such models. Even more so when using gradient-based methods, that can be carried out using a single GPU. In this era of abundance of information, making deep learning more accessible gives ample opportunity for positive societal impacts.

However, those advances are not without risk. Any research that makes learning from data easier and more accessible, risks aiding individuals and organizations with all sorts of intentions. Our work is no exception. Another particular concern stems from the fact that SSL makes it possible to learn from large datasets without annotations. As a result, the number of choices for training data expands. A non-careful choice of data may introduce bias and lead to biased systems.

References

[1] Cihang Xie, Mingxing Tan, Boqing Gong, Jiang Wang, Alan Yuille, and Quoc V. Le. Adversarial examples improve image recognition. In CVPR, 2020.
[2] Hugo Touvron, Andrea Vedaldi, Matthijs Douze, and Hervé Jégou. Fixing the train-test resolution discrepancy: Fixefficientnet, 2020.

[3] Ning Wang, Yang Gao, Hao Chen, Peng Wang, Zhi Tian, Chunhua Shen, and Yanning Zhang. Nas-fcos: Fast neural architecture search for object detection. In CVPR, 2020.

[4] Barret Zoph and Quoc V. Le. Neural architecture search with reinforcement learning. In International Conference on Learning Representations (ICLR), 2017.

[5] Esteban Real, Sherry Moore, Andrew Selle, Saurabh Saxena, Yutaka Leon Suematsu, Jie Tan, Quoc V. Le, and Alexey Kurakin. Large-scale evolution of image classifiers. In International Conference on Machine Learning (ICML), 2017.

[6] Esteban Real, Alok Aggarwal, Yanping Huang, and Quoc V. Le. Regularized evolution for image classifier architecture search. In International Conference on Machine Learning - ICML AutoML Workshop, 2018.

[7] Hanxiao Liu, Karen Simonyan, and Yiming Yang. Darts: Differentiable architecture search. In International Conference on Learning Representations (ICLR), 2019.

[8] Carl Doersch, Abhinav Gupta, and Alexei A. Efros. Unsupervised visual representation learning by context prediction. In The IEEE International Conference on Computer Vision (ICCV), December 2015.

[9] Richard Zhang, Phillip Isola, and Alexei A Efros. Colorful image colorization. In European conference on computer vision, pages 649–666. Springer, 2016.

[10] Mehdi Noroozi and Paolo Favaro. Unsupervised learning of visual representations by solving jigsaw puzzles. In European Conference on Computer Vision, pages 69–84. Springer, 2016.

[11] Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. arXiv preprint arXiv:2002.05709, 2020.

[12] Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross Girshick. Momentum contrast for unsupervised visual representation learning. In CVPR, 2020.

[13] Xinlei Chen, Haoqi Fan, Ross Girshick, and Kaiming He. Improved baselines with momentum contrastive learning. arXiv preprint arXiv:2003.04297, 2020.

[14] Yonglong Tian, Dilip Krishnan, and Phillip Isola. Contrastive multiview coding. arXiv preprint arXiv:1906.05849, 2019.

[15] Aaron van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. arXiv preprint arXiv:1807.03748, 2018.

[16] Hieu Pham, Melody Y Guan, Barret Zoph, Quoc V. Le, , and Jeff Dean. Efficient neural architecture search via parameter sharing. In International Conference on Machine Learning (ICML), 2018.

[17] Han Cai, Ligeng Zhu, and Song Han. Proxylessnas: Direct neural architecture search on target task and hardware. In ICLR, 2019.

[18] Asaf Noy, Niv Nayman, Tal Ridnik, Nadav Zamir, Sivan Doveh, Itamar Friedman, Raja Giryes, and Lihi Zelnik-Manor. Asap: Architecture search, anneal and prune. In arXiv:1904.04123, 2019.

[19] Hanwen Liang, Shifeng Zhang, Jiacheng Sun, Xingqiu He, Weiran Huang, Kechen Zhuang, and Zhenguo Li. Darts+: Improved differentiable architecture search with early stopping, 2019.

[20] Xin Chen, Lingxi Xie, Jun Wu, and Qi Tian. Progressive differentiable architecture search: Bridging the depth gap between search and evaluation. In Proceedings of the IEEE International Conference on Computer Vision, pages 1294–1303, 2019.

[21] Sirui Xie, Hehui Zheng, Chunxiao Liu, and Liang Lin. SNAS: stochastic neural architecture search. In International Conference on Learning Representations, 2019.
[22] M. Tan, B. Chen, R. Pang, V. Vasudevan, M. Sandler, A. Howard, and Q. V. Le. Mnasnet: Platform-aware neural architecture search for mobile. In 2019 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), pages 2815–2823, 2019.

[23] 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 2019 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), pages 10726–10734, 2019.

[24] Chenxi Liu, Liang-Chieh Chen, Florian Schroff, Hartwig Adam, Wei Hua, Alan Yuille, and Fei Fei Li. Auto-deeplab: Hierarchical neural architecture search for semantic image segmentation. In CVPR, 01 2019.

[25] Yu Weng, Tianbao Zhou, Yujie Li, and Xiaoyu Qiu. Nas-unet: Neural architecture search for medical image segmentation. In IEEE Access (Volume: 7 ), 2019.

[26] Zhuotun Zhu, Chenxi Liu, Dong Yang, Alan Yuille, and Daguang Xu. V-nas: Neural architecture search for volumetric medical image segmentation. In arXiv:1906.0281, 2019.

[27] Wang Ning, Gao Yang, Chen Hao, Wang Peng, Tian Zhi, and Shen Chunhua. Nas-fcos: Fast neural architecture search for object detection. In arXiv:1906.04423, 2019.

[28] Hanchao Wang and Jun Huan. Agan: Towards automated design of generative adversarial networks. In arXiv:1906.11080, 2019.

[29] Sivan Doveh, Eli Schwartz, Chao Xue, Rogerio Feris, Alex Bronstein, Raja Giryes, and Leonid Kailinsky. Metadapt: Meta-learned task-adaptive architecture for few-shot classification, 2019.

[30] Alex Krizhevsky. Learning multiple layers of features from tiny images, 2009.

[31] Deepak Pathak, Philipp Krahenbuhl, Jeff Donahue, Trevor Darrell, and Alexei A Efros. Context encoders: Feature learning by inpainting. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 2536–2544, 2016.

[32] Spyros Gidaris, Praveer Singh, and Nikos Komodakis. Unsupervised representation learning by predicting image rotations. arXiv preprint arXiv:1803.07728, 2018.

[33] Huan Xu and Shie Mannor. Robustness and generalization. In Machine Learning, 86(3):391–423, 2012.

[34] Weiyang Liu, Yandong Wen, Zhiding Yu, and Meng Yang. Large-margin softmax loss for convolutional neural networks. In Proceedings of the 33rd International Conference on International Conference on Machine Learning - Volume 48, ICML’16, page 507–516. JMLR.org, 2016.

[35] J. Sokolić, R. Giryes, G. Sapiro, and M. R. D. Rodrigues. Robust large margin deep neural networks. IEEE Transactions on Signal Processing, 65(16):4265–4280, Aug 2017.

[36] Peter L. Bartlett, Dylan J. Foster, and Matus Telgarsky. Spectrally-normalized margin bounds for neural networks. In Proceedings of the 31st International Conference on Neural Information Processing Systems, NIPS’17, page 6241–6250, Red Hook, NY, USA, 2017. Curran Associates Inc.

[37] Behnam Neyshabur, Srinadh Bhojanapalli, and Nathan Srebro. A pac-bayesian approach to spectrally-normalized margin bounds for neural networks. In ICLR, 2018.

[38] Behnam Neyshabur, Srinadh Bhojanapalli, David Mcallester, and Nati Srebro. Exploring generalization in deep learning. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems 30, pages 5947–5956. Curran Associates, Inc., 2017.

[39] Sanjeev Arora, Rong Ge, Behnam Neyshabur, and Yi Zhang. Stronger generalization bounds for deep nets via a compression approach. In Jennifer Dy and Andreas Krause, editors, Proceedings of the 35th International Conference on Machine Learning, volume 80 of Proceedings of Machine Learning Research, pages 254–263, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR.
[40] Jure Sokolic, Raja Giryes, Guillermo Sapiro, and Miguel Rodrigues. Generalization Error of Invariant Classifiers. In Aarti Singh and Jerry Zhu, editors, Proceedings of the 20th International Conference on Artificial Intelligence and Statistics, volume 54, pages 1094–1103, Fort Lauderdale, FL, USA, 20–22 Apr 2017.

[41] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In arXiv:1512.03385, 2015.

[42] Olga Russakovsky, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael Bernstein, et al. Imagenet large scale visual recognition challenge. International journal of computer vision, 115(3):211–252, 2015.

[43] Adam Coates, Andrew Ng, and Honglak Lee. An analysis of single-layer networks in unsupervised feature learning. In Proceedings of the fourteenth international conference on artificial intelligence and statistics, pages 215–223, 2011.

[44] Qizhe Xie, Eduard Hovy, Minh-Thang Luong, and Quoc V Le. Self-training with noisy student improves imagenet classification. arXiv preprint arXiv:1911.04252, 2019.

[45] Ekin D. Cubuk, Barret Zoph, Dandelion Mane, Vijay Vasudevan, and Quoc V. Le. Autoaugment: Learning augmentation policies from data. arXiv preprint arXiv:1805.09501v2, 2018.

[46] Sungbin Lim, Ildoo Kim, Taesup Kim, Chiheon Kim, and Sungwoong Kim. Fast autoaugment. In Advances in Neural Information Processing Systems (NeurIPS), 2019.