

Differentiable Architecture Search

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Abstract

Neural Architecture Search is a part of the AutoML field where a large number of various algorithms have emerged in recent years. One of the remarkable approaches is DARTS (Liu et al., 2019b), differentiable architecture search. In this work (Liu et al., 2019b), the authors managed to relax the discrete search space to the continuous one and applied gradient-based optimization to architecture cell search. The models learned with DARTS achieve competitive performance on several tasks while requiring sufficiently reduced computational cost. There are a lot of works improving some weaknesses of DARTS towards more accurate and efficient NAS algorithms. The goal of this project is to implement DARTS algorithm.

1. Introduction

The great success of deep learning models in various fields (Hsu et al., 2021), (Dosovitskiy et al., 2021) is often considered to be the result of automated process of feature engineering that replaced manual feature selection. At the same time, the research during the recent years showed the key importance of the deep architecture itself, that usually involves a huge amount of human efforts and expertise (Elsken et al., 2019), (Ren et al., 2020). Hence, the next level of abstraction is to automatize the process of neural architecture construction. The goal of Neural Architecture Search (NAS) is to automatically construct a neural architecture with high quality under the limited resources. The general pipeline of NAS is shown in the Figure 1. In recent years, a large number of NAS algorithms have emerged and achieved performance competitive with hand-crafted architectures. (Pham et al., 2018), (Wu et al., 2019), (Wen et al., 2020). However, one of the main problems of various approaches in this field is the cost of learning an architecture, i.e. computational time and resources (Liu et al., 2019b). Thus, a lot of works is aimed to make the process of architecture search more efficient. These approaches include well-designed search space (Liu et al., 2018b), weight inheritance (Cai et al., 2018), weight sharing (Pham et al., 2018). A fundamentally different approach is proposed in

the paper (Liu et al., 2019b). The general idea of DARTS (Liu et al., 2019b) is to make continuous relaxation of the search space, which allows to formulate the problem of NAS as differentiable task that can be solved via gradient-based optimization. The elegant solution proposed in DARTS algorithm is further developed in a series of subsequent works (Jiang et al., 2019), (Chen et al., 2019), (Dong & Yang, 2019), that obtain better results in terms of both task quality and computational cost.

1.1. General Problem Statement

The goal of this project is to implement the DARTS method and evaluate the learned model. More precisely, the project objectives include the choice of an appropriate convolutional architecture and a reasonable search space, implementations of one-level and bi-level optimization and evaluation of the learned architecture on a dataset of small size (e.g. CIFAR10, MNIST etc.).

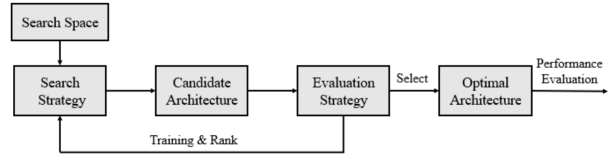


Figure 1. The general framework of NAS. NAS generally starts with a set of predefined operation sets, and uses search strategies to obtain a large number of candidate network architectures based on the search space formed by the operation sets. The candidate network architecture is trained and ranked. Then, the search strategy is adjusted according to the ranking information of the candidate network architecture, thereby further obtaining a set of new candidate network architectures. When the search is terminated, the most promising network architecture is used as the final optimal network architecture, which is used for the final performance evaluation (Ren et al., 2020).

2. DARTS: Differentiable Architecture Search

In this section, we describe the main aspects of the DARTS algorithm (Liu et al., 2019b): search space, continuous relaxation and optimization, approximate architecture gradient. This section is based on the formulation of DARTS

algorithm according to the original paper (Liu et al., 2019b).

2.1. Search Space

Following the previous works (Zoph et al., 2018), the authors of DARTS search for a computation cell as a structural element that forms the final architecture. It is possible to learn the cell to obtain a convolutional or a recurrent neural network. A cell is a directed acyclic graph (DAG) with N nodes: each node $x^{(i)}$ represents a latent representation, an operation $o^{(i,j)}$ that transforms $x^{(i)}$ is represented as an edge (i, j) . It is assumed that the cell has two input nodes, and the output of the cell is a concatenation of all the intermediate nodes. An intermediate node can be computed using the outputs of previous nodes:

$$x^{(j)} = \sum_{i < j} o^{(i,j)}(x^{(i)})$$

2.2. Continuous Relaxation and Optimization

The authors choose a set O of candidate operations (e.g., convolution, max pooling, etc.). To have continuous search space, instead of choosing one operation at a time, the authors propose to have a softmax over all possible operations (so called "mixed" operation):

$$\bar{o}^{(i,j)}(x) = \sum_{o \in O} \frac{\exp(\alpha_o^{(i,j)})}{\sum_{o' \in O} \exp(\alpha_{o'}^{(i,j)})} o(x)$$

The goal of DARTS is to learn the parameters $\alpha = \{\alpha^{(i,j)}\}$, where $\alpha^{(i,j)}$ has dimension $|O|$ for each pair (i, j) . When the training process of the cell is finished, final discrete architecture of the cell is obtained by replacing each mixed operation with the most probable operation according to the learned parameters α , i.e. $o^{(i,j)} = \arg \max_{o \in O} \alpha_o^{(i,j)}$.

DARTS jointly learns the architecture α and the weights w of operations. DARTS algorithm solves the bi-level optimization problem:

$$\min_{\alpha} L_{val}(w^*(\alpha), \alpha) \quad s.t. \quad w^*(\alpha) = \arg \min_w L_{train}(w, \alpha)$$

2.3. Approximate Architecture Gradient

Computation of architecture gradient is prohibitively expensive. Thus, the authors propose the following approximation

$$\nabla_{\alpha} L_{val}(w^*(\alpha), \alpha) \approx \nabla_{\alpha} L_{val}(w - \xi \nabla_w L_{train}(w, \alpha), \alpha)$$

where w denotes the weights on the current iteration, and ξ is the learning rate for a step of inner optimization. According to the chain rule, the approximate architecture gradient can be written as

$$\nabla_{\alpha} L_{val}(w', \alpha) - \xi \nabla_{\alpha, w}^2 L_{train}(w, \alpha) \nabla_{w'} L_{val}(w', \alpha)$$

where $w' = w - \xi \nabla_w L_{train}(w, \alpha)$. Since the expression above involves an expensive matrix-vector product, the authors propose to approximate it with finite difference:

$$\frac{\nabla_{\alpha, w}^2 L_{train}(w, \alpha) \nabla_{w'} L_{val}(w', \alpha) \approx \nabla_{\alpha} L_{train}(w^+, \alpha) - \nabla_{\alpha} L_{train}(w^-, \alpha)}{2\varepsilon}$$

where ε is a small scalar and $w^{\pm} = w \pm \varepsilon \nabla_w L_{val}(w', \alpha)$. This approximation reduces the complexity from $O(|\alpha||w|)$ to $O(|\alpha| + |w|)$.

When $\xi = 0$, the architecture gradient is given by $\nabla_{\alpha} L_{val}(w, \alpha)$. The authors note that while it leads to some acceleration in practice, its performance is worse. This setup is referred to as first-order approximation.

3. Literature Review

One of the most popular categorizations of the NAS research is given by the work (Elsken et al., 2019). According to (Elsken et al., 2019), mostly the NAS models vary in the three components: *search space*, *search strategy*, *performance estimation strategy*.

Search space determines the set of architectures that can be represented and learned by the particular NAS method. According to (Elsken et al., 2019), there are several typical choices of search spaces: chain-structured neural networks, multi-branch networks (Cai et al., 2018), networks consisting of repeated cells (Liu et al., 2019b).

Search strategy defines how to investigate the search space solving the conventional problem of "exploration vs exploitation". The main popular directions for search strategy are reinforcement learning (RL) (Zoph & Le, 2017), evolutionary algorithms (Real et al., 2018) and gradient-based optimization (Liu et al., 2019b), (Wu et al., 2019).

Performance estimation strategy refers to the task of candidate model's performance estimation on unseen data. The straightforward yet computationally expensive approach is to train the model from scratch and evaluate it on validation set. In practice, there are methods of reduced computation cost such as partial training (training for fewer epochs, on subset of data, etc.) (Zoph et al., 2018), weight sharing (candidate models are subgraphs of one large network) (Pham et al., 2018).

(Zoph & Le, 2017), one of the pioneering works in NAS, is based on reinforcement learning. In this approach, an agent builds the architecture sequentially layer by layer while the reward is the validation accuracy after training the model from scratch. The authors show that the learned models achieve performance comparable with the best performing networks, but the computational cost of search is extremely high.

In evolutionary search (Real et al., 2018), there is a set of population models and in each step, a parent model is sampled from population, and undergoes mutations to produce child networks. Mutations are some local operations (e.g., adding a layer of skip-connection) and the child networks are added to the population based on their estimated performance. The existing methods based on evolutionary search vary on the procedures of sampling parents, generating child networks and updating population (Elsken et al., 2019). The work (Real et al., 2019) compared the performance of RL-based algorithms and evolutionary algorithms, revealing that they perform almost equally in terms of test accuracy.

One of the remarkable works in gradient-based optimization is DARTS (Liu et al., 2019b). But there are other approaches towards continuous search space. For example, (Xie et al., 2019), (Cai et al., 2019b) use a parameterized distribution over the set of operations to perform gradient-based optimization, while (Shin et al., 2019) makes the relaxation similar to (Liu et al., 2019b) but over the set of a layer’s hyperparameters.

An important step in development of NAS is weight sharing trick (Bender et al., 2018) where the candidate models are sub-graphs of a larger model. The weights are shared and trained simultaneously. This technique is often used in different approaches, for example, as (Pham et al., 2018) and (Liu et al., 2019b).

A separate direction in NAS is to predict the model’s performance without training. For example, in TE-NAS (Chen et al., 2021) the authors exploit the eigenvalues in neural tangent kernel and the number of linear regions in the input space to construct the best performing model.

Recent research finds application of various algorithms to the NAS. For example, in AlphaNet (Wang et al., 2021), the authors incorporate knowledge distillation with α -divergence between the super-net as a teacher and sub-network as student into the training process. (Wang et al., 2021) with modifications show impressive performance according to (<https://paperswithcode.com/sota/neural-architecture-search-on-imagenet>).

3.1. DARTS: Pros and Cons

By the time the DARTS algorithm was proposed, the NAS had already reached the state-of-the-art performance in image classification task (Zoph et al., 2018), (Real et al., 2018). However, the computational cost to obtain those solutions was extremely high. For example, as argued by the authors of (Liu et al., 2019b), NAS with reinforcement learning (Zoph et al., 2018) required 2000 GPU days while the evolutionary algorithm (Real et al., 2018) required 3150 GPU days. High computational cost presents a severe problem for research in NAS field, especially in case of limited re-

sources or newcomers with little expertise. There are several works that propose to accelerate computations with various techniques such as well-designed search space (Liu et al., 2018b), inheritance of weights during training (Cai et al., 2018) or weight sharing (Pham et al., 2018). However, the main reason for scalability problem in many NAS approaches is that they mostly work in the statement of black-box optimization over a discrete domain. Thus, while the proposed approaches (Liu et al., 2018b), (Cai et al., 2018), (Pham et al., 2018) reduce computational burden having competitive or outperforming quality, they do not solve the problem in general. On the contrary, DARTS proposes a way to relax the discrete search space to be continuous which allows to replace the complicated black-box optimization with efficient gradient-based optimization. As a result, one of the main advantages of DARTS is sufficient reduction of computational cost while preserving highly competitive performance: it achieved high quality on CIFAR-10 dataset, competitive with the state-of-the-art performance of regularized evolution algorithm (Real et al., 2018) using three orders of magnitude less resources. Moreover, the authors (Liu et al., 2019b) showed high quality of DARTS approach when transferred a convolutional cell learned on CIFAR-10 dataset to ImageNet.

The work (Shin et al., 2019) explores the similar idea to relax the discrete search space to continuous form allowing differentiation. However, they do this not for the cell architecture itself but for hyperparameters of the layers, with main focus on hyperparameters of convolutional layers (i.e. filter size, number of channels, etc.). This may be seen as another advantage of DARTS that optimizes the structure of architecture cell and hence works with more complex and powerful search space.

There was another set of models (Saxenaa & Verbeek., 2016), (Ahmed & Torresani., 2017), (Veniat & Denoyer., 2018) that also followed the idea of search over continuous set but they restricted the architecture choice to some specific class. Thus, another important advantage is that DARTS is not limited to any particular model choice, and it is possible to learn the cell for both convolutional and recurrent network as a final architecture.

The work (Ren et al., 2020) defines some of the main disadvantages of the DARTS method. There are several approaches that attempt to eliminate the observed deficiencies of DARTS.

I-DARTS (Jiang et al., 2019). In DARTS approach, a node may be connected to several previous nodes. However, it is not possible to compare edges coming from different nodes and there should be only one edge between each pair of nodes in the final discretized architecture cell. This local mode of DARTS may result in sub-optimal solution. In the (Jiang et al., 2019) paper the authors propose to use softmax

over all incoming edges for a particular node, making it possible to compare all the incoming edges simultaneously. In practice, this allows to outperform DARTS with better convergence and faster training.

P-DARTS (Chen et al., 2019). Another known issue of DARTS is the "depth gap" (Chen et al., 2019) between the architectures during training and evaluation. Due to limited GPU memory, DARTS searches the cell structure in a shallow network (e.g., 8 cells) and evaluates the performance in a deeper networks (e.g., 20 cells). Since the cell was optimized in a smaller architecture, it may be no longer optimal for a deeper network. To alleviate this problem, the authors (Chen et al., 2019) propose P-DARTS to progressively increase the depth of the network during training of the cell. Having lower depth at the beginning of training allows to eliminate the operations with small weight on the later iterations. This helps to overcome the problem of increase in search space size with depth growth. According to the experiments, this approach achieves lower classification error on CIFAR10 and CIFAR100 and requires less amount of computational resources.

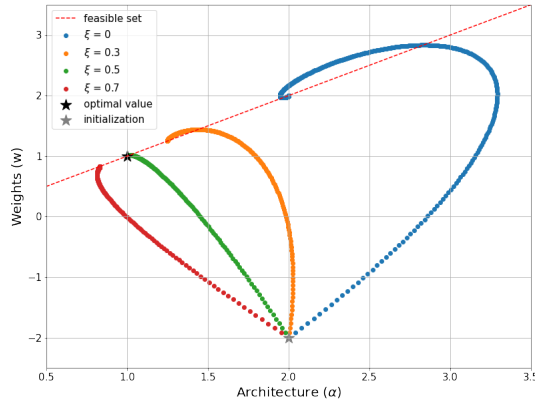


Figure 2. Reproducibility result for the toy experiment on bilevel optimization from the original paper (Liu et al., 2019b) (see Figure 2 in the original paper).

GDAS (Dong & Yang, 2019). In the (Dong & Yang, 2019), the authors point out two weaknesses of DARTS. First, DARTS uses outputs of all operations at each iteration and the cost to update all the parameters simultaneously is high. This also influences the total training time. Second, in simultaneous optimization, different operations can compete with each other, and this may lead to unstable optimization procedure. The GDAS (Dong & Yang, 2019) approach proposes to sample one sub-graph of the DAG at each iteration. In this case, each optimization step influences only part of a DAG, reducing unnecessary competition and accelerating the training process. According to the experimental results (Dong & Yang, 2019), GDAS is able to learn the model with performance comparable to DARTS but reduced

Table 1. Estimate of computational cost in terms of number of iterations (out of 10000) and time per iteration (sec).

	$\xi = 0$	$\xi = 0.3$	$\xi = 0.5$	$\xi = 0.7$
Number of iterations	659	411	296	335
Time per iteration	$4.4e - 4$	$9.0e - 4$	$9.1e - 4$	$9.3e - 4$

computation cost.

PC-DARTS (Xu et al., 2020). High memory consumption is another known issue of the DARTS algorithm. To alleviate this problem, PC-DARTS (Xu et al., 2020) approach samples the channels and convolves the sampled channel features. Instability may be a side effect of this procedure, thus, (Xu et al., 2020) also applies edge normalization to make the optimization more efficient. PC-DARTS sufficiently outperforms the baseline DARTS both in terms of search time and accuracy.

DARTS aroused interest in the NAS community, and there are more methods based on DARTS (Li et al., 2020), (Chen & Hsieh, 2020) or similar ideas (Wu et al., 2019), (Cai et al., 2019a), (Liu et al., 2019a).

4. Experiments

4.1. Example of bilevel optimization

First, we reproduce the toy experiment on bilevel optimization. Following the experiment from the original paper (Liu et al., 2019b) (see Figure 2 in the original paper), we use:

$$L_{\text{train}}(w, \alpha) = w^2 - 2\alpha w + \alpha^2, \quad (1)$$

$$L_{\text{val}}(w, \alpha) = \alpha w - 2\alpha + 1, \quad (2)$$

where w is the lower-level variable and α is the upper-level variable. Optimization starts from the initialization $(\alpha^{(0)}, w^{(0)}) = (2, -2)$. Analytical solution to this bilevel optimization problem is $(\alpha^*, w^*) = (1, 1)$. Also, there is a feasible set (given by equation $w(\alpha) = \alpha$) where the constraint on w holds exactly. We follow the algorithm of approximate bilevel optimization presented in the original paper (Liu et al., 2019b) (for simplicity, we used gradient descent without momentum) and reproduce the results. In this experiment, we use the learning rate $1e - 2$, maximal number of iterations 10000, the threshold $t = 1e - 4$. Optimization stops when either the maximal number of iterations is exceeded or both the deviations of w and α on the adjacent iterations is smaller than threshold: $|\alpha^{(i+1)} - \alpha^{(i)}| < t$ and $|w^{(i+1)} - w^{(i)}| < t$.

Similar to (Liu et al., 2019b), we plot the optimization trajectories for several choices of the hyperparameter ξ , see

Figure 2. Also, we estimate the optimization time / number of iterations to reach stop criteria for each value of ξ , see Table 1.

We can note that for all values of ξ the algorithm converges at least to the feasible set. Optimal value of ξ seems to be close to 0.5 and results in the shortest optimization trajectory (in terms of number of iterations) and most accurate solution. Moving away from the optimal value of ξ , we obtain longer convergence and less accurate results. From Table 1 we obtain that time per iteration for the first-order approximation (i.e. $\xi = 0$) is almost twice smaller than for the second-order approximation ($\xi > 0$). Our results are consistent with the paper (Liu et al., 2019b) outcomes.

4.2. Neural Architecture Search

Operations. Following (Liu et al., 2018a), we use the following set of operations: separable convolutions with kernel sizes 3×3 (padding 1) and 5×5 (padding 2), dilated separable convolutions with kernel sizes 3×3 (padding 2) and 5×5 (padding 4), max pooling and average pooling with kernel size 3×3 (both with padding 1), identity and zero operation. Padding is used to preserve spatial dimensions of output of each operation. According to (Liu et al., 2019b), we apply separable convolutions twice and enclose convolutions with ReLU and BathNorm.

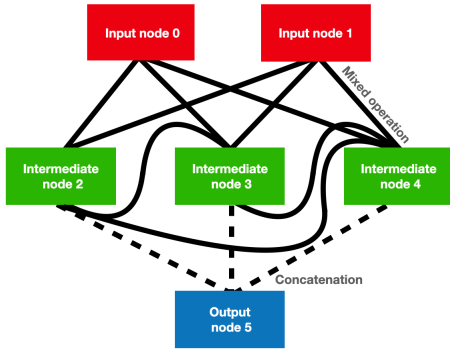


Figure 3. The cell architecture that we use in the experiments. The two red nodes are the input nodes; the three green nodes are the intermediate nodes; the blue node is the output node. Solid lines correspond to mixed operations between nodes; dash lines correspond to concatenation of the intermediate nodes’ outputs.

Cell. In the previous works (Liu et al., 2019b), (Liu et al., 2018a), the authors typically use two types of cells – normal and reduction cells. While the general architecture of both cells is the same, normal cell preserves spatial dimensions and reduction cell decreases spatial dimensions. In practice, this is achieved by using stride 1 in all operations of a normal cell and stride 2 in operations adjacent to the input nodes of a reduction cell. While we generally follow the architecture of a cell given in (Liu et al., 2019b), we slightly reduce the

number the nodes and the overall cell architecture is shown in Figure 3.

Shape adjustment. There are two issues related to the shapes mismatch. First, the number of output channels in the preceding cell may be incompatible with the number of input channels in the subsequent cell. This issue is usually solved by applying convolutions (Liu et al., 2018a) with kernel size 1×1 and stride 0, accompanied with ReLU and BatchNorm. Another shape mismatch occurs after applying reduction cell: due to decreased spatial dimensionality, there is a need to adjust spatial shape of another input as well. In this case, two convolutions are applied (Liu et al., 2018a). Each convolution acts on a separate spatial part of the input, and the output number of channels is divided in half between these convolutions. ReLU and BatchNorm are also applied here.

Network. Inspecting the works (Liu et al., 2018a), (Liu et al., 2019b), (Real et al., 2018), we observe that the conventional approach is to repeat blocks of several normal cells and a single reduction cell to form the network for architecture search. Thus, we use similar model, schematically shown in Figure 4. We use 8 layers in total, 2 normal cells alternating with a reduction cell. We also apply additional intermediate layers to force shapes’ compatibility. Initial number of channels is set to 16. We add a classifier on top of the last normal cell.

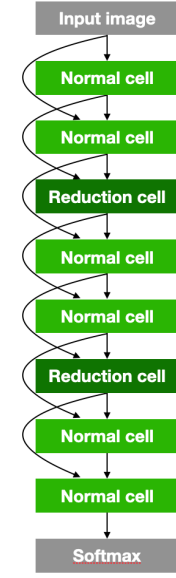


Figure 4. Network for architecture search that is used in our experiments.

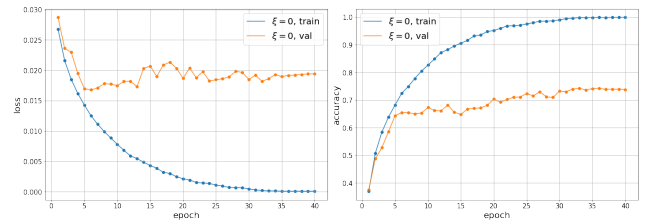


Figure 5. Training progress for cell architecture search with $\xi = 0$.

Training details. We largely follow the setup from (Liu et al., 2019b). We set batch size to 64 and train the model for 40 epochs. For model parameters w , we use SGD with initial learning rate 0.025 decreasing down to zero according to cosine annealing schedule, momentum 0.9 and weight

decay $3e-4$. For parameters α we use Adam optimizer with learning rate $3e-4$, weight decay $1e-3$, $\beta = (0.5, 0.999)$. We have zero initialization for α to provide uniform distribution over operations at the beginning of training. Cell architecture search is performed on the CIFAR10 dataset.

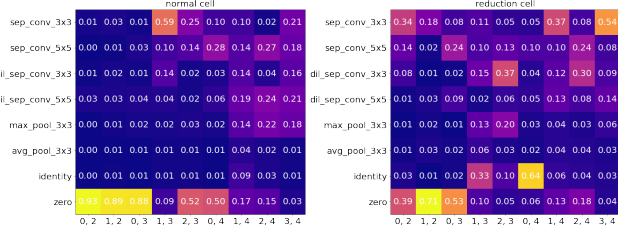


Figure 6. Values of α_{normal} , $\alpha_{\text{reduction}}$ at the end of training for cell architecture search with $\xi = 0$. X-axis corresponds to edges between nodes, Y-axis corresponds to operations.

Results. We first provide experiment with $\xi = 0$. Figure 5 shows that after training the model achieves $8.5e-05$ training loss and training accuracy of 0.99. At the same time, both validation loss and validation accuracy convergence slows down after 5 epochs. Final validation accuracy is 0.74. In Figure 6 we show the values of α_{normal} , $\alpha_{\text{reduction}}$ at the end of training (after softmax is applied). We note that there are several edges for which the zero operation has very high probability. We discretize the learned architecture according to method described in (Liu et al., 2019b): for each intermediate node, we choose top-2 operations from distinct preceding nodes (excluding zero operation) with the highest probabilities. For the corresponding normal and reduction cells see Figure 7.

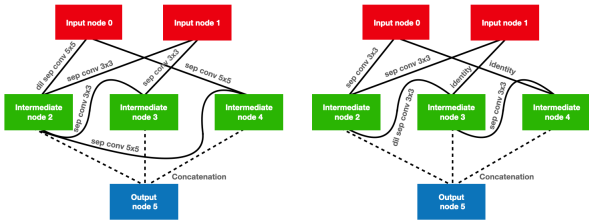


Figure 7. The learned architectures of normal (left) and reduction (right) cells when $\xi = 0$.

5. Future work

In the future work, we will conduct an experiment with $\xi > 0$. This will allow to compare the two regimes ($\xi = 0$ and $\xi > 0$) of bilevel optimization not only in terms of computational cost but also by visualizing the learned cell architectures in both cases. Further, we will train a final architectures consisting of the learned cells and analyze the performance it both cases. Current implementation of

DARTS and example experiments can be found here.¹

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¹https://github.com/VoronkovaDasha/project_darts

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