

## PA&DA: Jointly Sampling PAth and DAta for Consistent NAS

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Paper: https://arxiv.org/abs/2302.14772 Code: https://github.com/ShunLu91/PA-DA

Tag: <u>WED-AM-354</u>

## **1 Background & Motivation**





1.1 One-shot Neural Architecture Search (NAS)





# **1 Background & Motivation**





#### **1.2 Problem in One-Shot NAS**

- **Prombel** : shared weights suffer from different gradient descent directions
- Available solutions :
  - Elaborate a better path sampling strategy
    - FairNAS [ICCV'21], Magic-AT [ICML'22]
  - Maintain multi-copies of supernet weights
    - Few-Shot-NAS [ICML'21], GM [ICLR'22], CLOSE [ECCV'22]
  - Introduce additional loss regularizations
    - NSAS [CVPR'20] , SUMNAS [ICLR'22], Magic-AT [ICML'22]
  - Drawbacks : require multiple computation burdens and obtain unsatisfying results
- Motivate us to explore a better solution.





#### 2.1 Observations

- **Kendall's Tau (KT)**: we calculate the correlation between predicted scores and ground-truth scores of sub-models, to indicate the ranking consistency of sub-models.
- Gradient Variance (GV): we record the average GV of all candidate operation weights during training



- With more sub-models sharing weights, GV increases and KT becomes worse
- When using different methods, GV decreases and KT becomes better
- **Prompts**: reduce GV to improve the ranking consistency KT.



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#### 2.1 Observations



**Figure 1: Nonpriority and priority training examples for image classification.** *Left:* Examples that RAIS samples infrequently during training. *Right:* Examples that RAIS prioritizes. Bold denotes the image's label. Parentheses denote a different class that the model considers likely during training. Datasets are CIFAR-10 (top), CIFAR-100 (middle), and rotated MNIST (bottom).

 Inspiration from RAIS [NeurIPS'18]: better data sampling strategy can reduce the gradient variance of model training, thereby improving the generalization of the model.



#### 2.2 Traditional Sampling-based One-Shot NAS



• Stage 1: Supernet Training

$$\mathcal{W}^{\star} = \underset{\mathcal{W}}{\operatorname{argmin}} \mathbb{E}_{\substack{\alpha \sim \mathbf{p}(\mathcal{A}) \\ (x,y) \sim \mathbf{q}(\mathbb{D}_{T})}} [\mathcal{L}(\mathcal{N}(x,\alpha;\mathcal{W}_{\alpha}),y)] \quad (1)$$

• Stage 2: Sub-model Search

$$\alpha^{\star} = \operatorname*{argmax}_{\alpha \in \mathcal{A}} \mathbb{E}_{(x,y) \sim \mathbf{q}(\mathbb{D}_V)} [\mathcal{P}(\mathcal{N}(x,\alpha;\mathcal{W}_{\alpha}^{\star}),y)] \quad (2)$$





#### 2.3 Importance Sampling One-Shot NAS



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• Formulation of our objective: jointly optimize path and data sampling distribution during supernet training.

$$\mathcal{W}^{\star} = \underset{\mathcal{W}}{\operatorname{argmin}} \mathbb{E}[\mathcal{L}(\mathcal{N}(x, \alpha; \mathcal{W}_{\alpha}), y)]$$
s.t.
$$\begin{cases} \alpha \sim \mathbf{p}^{\star}(\mathcal{A}), \ (x, y) \sim \mathbf{q}^{\star}(\mathbb{D}_{T}), \\ \mathbf{p}^{\star} = \underset{\mathbf{q}}{\operatorname{argmin}} \mathbb{V}[d(\mathbf{p})], \\ \mathbf{q}^{\star} = \underset{\mathbf{q}}{\operatorname{argmin}} \mathbb{V}[d(\mathbf{q})] \end{cases}$$
(3)







• Supernet training in sampling-based one-shot NAS :

$$\mathcal{W}^{\star} = \underset{\mathcal{W}}{\operatorname{argmin}} \mathbb{E}_{\substack{\alpha \sim \mathbf{p}(\mathcal{A}) \\ (x,y) \sim \mathbf{q}(\mathbb{D}_{T})}} [\mathcal{L}(\mathcal{N}(x,\alpha;\mathcal{W}_{\alpha}),y)] \quad (1)$$

• PA&DA-Jointly optimize path and data sampling distribution during training:

$$\mathcal{W}^{\star} = \underset{\mathcal{W}}{\operatorname{argmin}} \mathbb{E}[\mathcal{L}(\mathcal{N}(x, \alpha; \mathcal{W}_{\alpha}), y)]$$
s.t.
$$\begin{cases} \alpha \sim \mathbf{p}^{\star}(\mathcal{A}), \ (x, y) \sim \mathbf{q}^{\star}(\mathbb{D}_{T}), \\ \mathbf{p}^{\star} = \underset{\mathbf{q}}{\operatorname{argmin}} \mathbb{V}[d(\mathbf{p})], \\ \mathbf{q}^{\star} = \underset{\mathbf{q}}{\operatorname{argmin}} \mathbb{V}[d(\mathbf{q})] \end{cases}$$
(3)





#### 2.4 PAth Importance Sampling (PA)



• At *i*-th training step, the stochastic gradient is:

$$d_i(p_i) = \frac{1}{Np_i} \nabla_{\mathcal{W}} \mathcal{L}(\mathcal{N}(x_i, \alpha_i; \mathcal{W}_{\alpha_i}), y_i)$$
(5)

• Introduce the gradient to our objective:

$$\min_{\mathbf{p}} \mathbb{V}[d(\mathbf{p})] = \mathbb{E}\left[d^{\top}d\right] - \mathbb{E}\left[d\right]^{\top} \mathbb{E}\left[d\right]$$
(6)

• Reformulate the problem in Eq.6 as a constrained optimization problem:

$$\begin{split} \min_{\mathbf{p}} \sum_{i=1}^{N} \frac{1}{N^2} \frac{1}{p_i} \left\| \nabla_{\mathcal{W}} \mathcal{L}(\mathcal{N}(x_i, \alpha_i; \mathcal{W}_{\alpha_i}), y_i) \right\|^2 \\ \text{s.t.} \sum_{i=1}^{N} p_i = 1 \quad \text{and} \quad p_i \geq 0 \quad \forall i = 1, 2, \dots N \end{split}$$

• Use the Lagrange multiplier method to solve the optimal path sampling distribution:

$$p_i^{\star} = \frac{\|\nabla_{\mathcal{W}} \mathcal{L}(\mathcal{N}(x_i, \alpha_i; \mathcal{W}_{\alpha_i}), y_i)\|}{\sum_{i=1}^N \|\nabla_{\mathcal{W}} \mathcal{L}(\mathcal{N}(x_i, \alpha_i; \mathcal{W}_{\alpha_i}), y_i)\|}$$
(10)

• Conclusion: the optimal  $p_i^*$  is proportional to the normalized gradient norm of the sub-model.





#### 2.5 DAta Importance Sampling (DA)



• According to previous works, the optimal data sampling distribution  $q_i^*$  is given by:

$$q_i^{\star} \propto \|\nabla_{\mathcal{W}} \mathcal{L}(\mathcal{N}(x_i, \alpha_i; \mathcal{W}_{\alpha_i}), y_i)\|$$
(11)

- In mini-batch training, it is time-consuming and laborious to compute per-sample gradient norm. Thereby we use the Upper-bound [ICML'18] method to approximate:
   sup{||∇<sub>W</sub> L(N(x<sub>i</sub>, α<sub>i</sub>; W<sub>α<sub>i</sub></sub>), y<sub>i</sub>)||} ≤ ||∇<sub>L</sub>|| (12)
- For image classification with a cross-entropy loss, the approximated upper bound is:

$$7_L = \operatorname{softmax}(y_L) - \mathbb{1}(y_i) \tag{13}$$

 In this way, we can efficiently approximate the gradient norm of each sample via a batch-wise mannar.







#### 2.6 Supernet training in practice

Algorithm 1 Supernet training algorithm of PA&DA Input: Input training data  $\mathbb{D}_T$ , supernet  $\mathcal{N}$  with weights  $\mathcal{W}$ , training epochs  $n_{epochs}$ , training steps  $n_{steps}$  per epoch. Output: Optimized supernet weights  $\mathcal{W}^*$ .

- 1: for j = 1 to  $n_{epochs}$  do
- 2: for k = 1 to  $n_{steps}$  do
- 3: Sample a path based on the distribution  $\mathbf{p}(\mathcal{A})$ ;
- 4: Sample a mini-batch training data based on the distribution  $\mathbf{q}(\mathbb{D}_T)$ ;
- 5: Train supernet weights  $\mathcal{W}$  by gradient descent;
- 6: Record gradient norm of the sampled path after back-propagation;
- 7: Approximate and record gradient norm of the sampled data using Eq.13.
- 8: end for
- 9: Linearly increase smoothing parameters  $\delta$  and  $\tau$ ;
- 10: Update the path sampling distribution  $\mathbf{p}(\mathcal{A})$  according to Eq.10 and add it to uniform distribution;
- 11: Update the data sampling distribution  $\mathbf{q}(\mathbb{D}_T)$  according to Eq.11 and add it to uniform distribution;
- 12: **end for**

- Path importance sampling:
  - Update the path sampling distribution after each epoch.
  - To handle those parameter-free operations, employ a smoothing parameter δ to add path importance sampling distribution and the uniform sampling distribution together.
- Data importance sampling:
  - Update the data sampling distribution after each epoch.
  - To handle those data not sampled in the current epoch, employ a smoothing parameter τ to add data importance sampling distribution and the uniform sampling distribution.



### **3 Experiments**





#### 3.1 Ranking Consistency in NAS-Bench-201 using CIFAR-10

Method	Cost	KT	P@Top5%
SPOS [16]	1.6	$0.639 \pm 0.030$	$0.211\pm0.168$
FairNAS <sup>†</sup> [7]	5.4	$0.541\pm0.023$	$0.160\pm0.034$
Magic-AT <sup>†</sup> [46]	4.4	$0.547\pm0.059$	$0.019\pm0.011$
NSAS [48]	14.6	$0.653\pm0.051$	$0.064\pm0.028$
SUMNAS <sup>†</sup> [17]	22.6	$0.505\pm0.039$	$0.145\pm0.061$
Few-Shot-25 [51]	18.6	0.696	-
GM <sup>†</sup> -8 [ <mark>18</mark> ]	18.0	$0.656\pm0.011$	$0.153\pm0.006$
CLOSE [52]	2.5	$0.643\pm0.050$	$0.031\pm0.021$
PA&DA	1.8	$\textbf{0.713} \pm \textbf{0.002}$	$\textbf{0.301} \pm \textbf{0.018}$

 PA&DA only consumes 1.8 GPU hours and reaches the highest KT and P@Top5%.



 Supernet trained by PA&DA has the lowest GV and the highest KT.







#### **3.2 Search performance in DARTS using CIFAR-10**

Method	<b>Test Accuracy</b>		Parameters	Search Cost	Search
	Best(%)	Average(%)	<b>(M)</b>	(GPU Days)	Method
NASNet-A [59]	97.35	-	3.3	1,800	RL
ENAS [34]	97.11		4.6	0.5	RL
DARTS [30]	-	$97.00\pm0.14$	3.3	0.4	Gradient
GDAS [14]	97.07	- 1939	3.4	0.3	Gradient
RandomNAS [28]	-	$97.15\pm0.08$	4.3	2.7	Random
DARTS-PT [46]	97.52	$97.39\pm0.08$	3.0	0.8	Gradient
BaLeNAS [54]		$97.50\pm0.07$	3.8	0.6	Gradient
AGNAS [42]	97.54	$97.47\pm0.003$	3.6	0.4	Gradient
ZARTS [47]	-	$97.46 \pm 0.07$	3.7	1.0	Gradient
GDAS-NSAS [53]	97.27	- 19	3.5	0.4	Gradient
RandomNAS-NSAS [53]	97.36		3.1	0.7	Random
Few-Shot-NAS <sup>†</sup> [56]	97.42	$97.37\pm0.06$	3.8	2.8	Gradient
GM [20]	97.60	$97.51 \pm 0.08$	3.7	2.7	Gradient
CLOSE [57]		$97.28\pm0.04$	4.1	0.6	Gradient
PA&DA	97.66	$\textbf{97.52} \pm \textbf{0.07}$	3.9	0.4	Random

Table 2. Comparison with other state-of-the-art methods on the CIFAR-10 dataset using DARTS search space. We report the best and average test accuracy of repeated experiments.<sup>†</sup>: reported by GM [20].

• PA&DA only consumes 0.4 GPU days and achieves the best performance.





#### 3.2 Searched architectures in DARTS using CIFAR-10





### **3 Experiments**





#### **3.3 Search performance in ProxylessNAS on ImageNet**

Method	Params. (M)	FLOPs (M)	Top-1 (%)	Top-5 (%)
AmoebaNet-A [35]	5.1	555	74.5	92.0
MnasNet-A1 [43]	3.9	312	75.2	92.5
PNAS [29]	5.1	588	74.2	91.9
TNASP-C [32]	5.3	497	75.8	92.7
DA-NAS [12]	- 696	389	74.6	- 1. S
SPOS [18]	5.4	472	74.8	-
FBNet-C [48]	5.5	375	74.9	- 25
ProxylessNAS [4]	7.1	465	75.1	92.3
FairNAS-A [9]	4.6	388	75.3	
MAGIC-AT [50]	6.0	598	76.8	93.3
Few-Shot NAS [56]	4.9	521	75.9	-
GM [20]	4.9	530	76.6	93.0
PA&DA	5.3	399	77.3	93.5

Table 3. Comparison with other state-of-the-art methods on theImageNet dataset using the ProxylessNAS search space.

• PA&DA obtains the SOTA performance while using similar FLOPs.





#### Conclusion

- In this paper, we observe that large gradient variance during supernet training harms the ranking consistency.
- Then we derive the relationship between the gradient variance and the sampling distributions.
- Finally, we reduce the gradient variance for the supernet training by jointly optimizing the path and data sampling distributions to improve the supernet ranking consistency.

- Future Work
  - Explore more effective metrics for data importance.
  - Concentrate more on sub-models located in the Pareto-front, rather than exhaustively evaluate all sub-models.







