Multi-fidelity Neural Architecture Search with Knowledge Distillation

Ilya Trofimov\textsuperscript{1}, Nikita Klyuchnikov\textsuperscript{1}, Mikhail Salnikov\textsuperscript{1}, Alexander Filippov\textsuperscript{2}, and Evgeny Burnaev\textsuperscript{1}

\textsuperscript{1} Skolkovo Institute of Science and Technology, Moscow, Russia
\textsuperscript{2} Huawei Noah’s Ark Lab, Moscow, Russia

Abstract. Neural architecture search (NAS) targets at finding the optimal architecture of a neural network for a problem or a family of problems. Evaluations of neural architectures are very time-consuming. One of the possible ways to mitigate this issue is to use low-fidelity evaluations, namely training on a part of a dataset, fewer epochs, with fewer channels, etc. In this paper, we propose a bayesian multi-fidelity method for neural architecture search: MF-KD. The method relies on a new approach to low-fidelity evaluations of neural architectures by training for a few epochs using a knowledge distillation. Knowledge distillation adds to a loss function a term forcing a network to mimic some teacher network. We carry out experiments on CIFAR-10, CIFAR-100, and ImageNet-16-120. We show that training for a few epochs with such a modified loss function leads to a better selection of neural architectures than training for a few epochs with a logistic loss. The proposed method outperforms several state-of-the-art baselines.

Keywords: Neural Architecture Search · Multi-fidelity Optimization · Bayesian Optimization · Knowledge Distillation

1 Introduction

Deep learning is state of the art in the majority of ML problems: computer vision, speech recognition, machine translation, etc. The progress in this area mostly comes from discovering new architectures of neural networks, which is usually performed by human experts. This motivates a new direction of research – neural architecture search (NAS) – developing algorithms for finding new well-performing architectures of neural networks. Existing approaches could be broadly divided into two groups.

Black-box optimization. Given a discrete search space $\mathcal{A}$ of all the architectures and a performance function $f(\cdot)$ of an architecture, like testing accuracy, these approaches aim to solve $\arg\max_{a \in \mathcal{A}} f(a)$ via black-box optimization. One of the first proposed approaches of this kind \cite{zoph,baker} treated architecture design (layer by layer) as a sequential decision process and the performance $f(a)$ was a reward. The optimization was done by reinforcement learning. Classical methods like Gaussian process-based bayesian optimization with a particular kernel \cite{srinivas}
and evolutionary optimization also could be applied. Some methods use performance predictors together with bayesian uncertainty estimation. The black-box optimization methods share the same drawback – they require a large number of architecture evaluations and significant computational resources.

**One-shot NAS.** Another line of research goes beyond black-box optimization and utilizes the structure and the learning algorithm of a neural network. The architecture search is done simultaneously with the training of networks themselves, and the search time is not significantly larger than a training time of one network. The key idea of the one-shot NAS is the *weight-sharing* trick – that is, all the architectures from the search space share weights of architecture blocks. Some black-box methods like evolutionary search and RL-based NAS can be modified by the weight-sharing and enjoy considerable speedup.

The DARTS method considers a supernetwork containing all the networks from a search space as its subnetworks. The choice between subnetworks is governed by architectural parameters which are updated by gradient descent similarly to differentiable hyperparameters optimization methods. Subsequent modifications improve DARTS in terms of search speed and performance of resulting architectures. Alternative approaches update subnetworks randomly during the training phase. Then, the best subnetwork is selected by its validation accuracy.

Overall, black-box optimization methods are much slower but more robust and general. Given a rich search space of architectures, a black-box method typically will find a good one though spending a lot of time. Also black-box optimization doesn’t restrict the network’s performance to be differentiable with respect to architectural parameters, like DARTS. Constraints like FLOPS/latency/memory footprint can be applied straightforwardly. Popular one-shot methods like DARTS
and ENAS are quite fast. Unfortunately, they perform only slightly better than the random search \[43,1,22\].

Is it possible to speedup black-box NAS? The natural approach is to do low-fidelity evaluations of neural architectures, for example, train them for a few epochs. However, the final goal is to find the best architecture in terms of a high-fidelity evaluation — after training until convergence. An interesting research question arises: is it possible to make correct architecture selection after training for a few epochs? Obviously, this selection is not perfect, but we show how to improve it by training with a knowledge distillation (KD) loss function. We found that the proposed technique not only improves the accuracy of a network but also improves the correlation between low- and high-fidelity evaluations.

In this paper, we make the following contributions:

– we propose a new approach to the low-fidelity evaluation of neural architectures — training for a few epochs with a knowledge distillation loss (Section 3.2);
– we incorporate the proposed low-fidelity evaluations into a bayesian multi-fidelity search method “MF-KD” based on co-kriging (Figure 1 and Section 3.3);
– we carry out experiments with the NAS-Bench-201 benchmark \[8\], including CIFAR-10, CIFAR-100, and ImageNet-16-120. We prove that the proposed approach leads to the better architecture selection, given the same computational budget, than several state-of-the-art baselines (Section 4);

The code is in the repository
\[https://anonymous.4open.science/r/a6c96420-435a-484b-9170-e2de9ab0ae3/\]

2 Related Work

Knowledge distillation (KD) was proposed in \[11\]. The seminal paper matched predictions of a student and a teacher with cross-entropy. Later extensions suggest matching features maps instead of class probabilities \[33,45,39,30,2,28,12,38\]. The methods similar to KD were developed for other problems: sequences-to-sequence modeling \[17\], reinforcement learning \[34\], etc.

Multi-fidelity/low-fidelity. Low-fidelity evaluations are used sometimes in the context of hyperparameter optimization and NAS. The proposed variants include: training on a part of dataset \[18\], shorter training time \[46\], lower resolution of images \[6\], less filters per payer \[48\]. Low-fidelity evaluations are faster but they are biased. This issue motivates multi-fidelity methods which progressively increase fidelity during the search: MF-GP-UCB \[13\], MF-MI-Greedy \[37\], co-kriging \[19\].

KD & NAS. Some very recent papers study applications of KD to NAS. \[21\] propose to independently train blocks in a student’s supernetwork by mimicking corresponding blocks of a teacher with MSE loss. \[15\] proposed an oracle
knowledge distillation loss and showed that ENAS \cite{31} with this loss outperforms ENAS with logistic loss. \cite{26} studies RL-based NAS with networks trained with KD loss instead of a logistic loss. They conclude that the found architecture depends on the teacher architecture used for KD, that is, some structural knowledge is transferred from a teacher.

The main difference between our work and the aforementioned papers is that we use KD loss for improving low-fidelity evaluations of architectures — inside a multi-fidelity search algorithm. At the same time, \cite{26} does only high-fidelity evaluations (training on the full dataset). \cite{15,21} incorporates KD loss into training of a supernetwork, while our work is about treating NAS as a search over a discrete domain of architectures.

3 The proposed method

3.1 Knowledge Distillation (KD)

The knowledge distillation (KD) assumes two models: a teacher and a student. The teacher is typically a large and accurate network or an ensemble. The student is trained to fit the softmax outputs of the teacher together with ground truth labels. The idea is that outputs of the teacher capture not only the information provided by ground truth labels but also the probabilities of other classes — “dark knowledge”. The knowledge distillation can be summarized as follows.

Let \( z_i \) be logits (pre-softmax activations) and \( q_i \) — probabilities of classes as predicted by a neural network. Knowledge distillation smooths \( z_i \) with the temperature \( \tau \)

\[
q_i = \sigma(z_i/\tau) = \frac{\exp(z_i/\tau)}{\sum_j \exp(z_j/\tau)},
\]

(1)

Neural networks often do very confident predictions (close to 0 or 1) and smoothing helps to provide for student more information during training \cite{11}. The KD loss is a linear combination of the logistic loss and cross-entropy between predictions of the teacher and the student

\[
(1 - \lambda) \sum_i H(y_i, \sigma(z_i^S)) + \lambda \tau^2 \sum_i H(\sigma(z_i^T/\tau), \sigma(z_i^S/\tau)),
\]

(2)

where \( z_i^T, z_i^S \) are logits of the teacher and the student, \( H(p, q) = -p \log(q) \) is the cross-entropy function. The factor \( \tau^2 \) is used for scaling gradients of both parts of the loss function to be the same order. In the rest of the paper, we will refer to this variant of the knowledge distillation as “original KD”.

Other variants of KD suggest matching feature maps of the student and the teacher with various discrepancy functions \cite{33,15,39,30,28,12,38}. For example, the NST loss \cite{12} uses Maximum Mean Discrepancy (MMD):

\[
\sum_i \left( H(y_i, \sigma(z_i^S)) + \beta \mathcal{L}_{MMD^2}(F_iT, F_iS) \right),
\]

(3)
where $F_T$, $F_S$ are the feature maps of the teacher and the student,

$$L_{MMD^2}(F^T, F^S) = \frac{1}{C^T_T} \sum_{i=1}^{C_T} \sum_{i' = 1}^{C_T} k(\frac{f^i_T}{||f^i_T||_2}, \frac{f^{i'}_T}{||f^{i'}_T||_2}) + \frac{1}{C^S_S} \sum_{j=1}^{C_S} \sum_{j' = 1}^{C_S} k(\frac{f^j_S}{||f^j_S||_2}, \frac{f^{j'}_S}{||f^{j'}_S||_2})$$

$$- \frac{2}{C_TC_S} \sum_{i=1}^{C_T} \sum_{j=1}^{C_S} k(\frac{f^i_T}{||f^i_T||_2}, \frac{f^j_S}{||f^j_S||_2}).$$

(4)

Here $f^i_T, f^j_S$ are feature maps from the layers $i, j$ of the teacher and the student respectively, $k(x, y)$ is a kernel.

### 3.2 Low-fidelity evaluations with knowledge distillation

Let $\alpha$ be an architecture from a search space $A$. We assume that each architecture could be represented by a real-valued vector of features $x \in X \subseteq \mathbb{R}^d$. We call $y(x)$ an evaluation of the architecture $\alpha$, namely its validation accuracy after fitting on the train dataset. We use the following notations:

- $y^1(x)$ - low-fidelity evaluation, that is, validation accuracy of the network $\alpha$ after fitting on the train dataset for $E_1$ epochs with the NST loss (3);
- $y^2(x)$ - high-fidelity evaluation, that is, validation accuracy of the network $\alpha$ after fitting on the train dataset for $E_2$ epochs with the logistic loss, $E_2 > E_1$.

The better low-fidelity evaluation $y^1(x)$ is, the higher a correlation between $y^1(x)$ and $y^2(x)$ should be. Even when correlation is large, low-fidelity evaluations are not enough since typically they are biased:

$$\text{argmax}_x y^1(x) \neq \text{argmax}_x y^2(x).$$

(5)

This bias motivates multi-fidelity search methods that combine low- and high-fidelity evaluations.

### 3.3 Multi-fidelity NAS

We combine low-fidelity $y^1(x)$ and high-fidelity $y^2(x)$ evaluations via the co-kriging fusion model

$$y^2(x) = \rho y^1(x) + \delta(x),$$

(6)

where $y^2(x)$, $y^1(x)$, $\delta(x)$ are Gaussian Processes [11], $y^1(x)$ is independent of $\delta(x)$, in turn, $\delta(x)$ allows handling biases [5], $\rho$ is a scaling factor which is fitted by maximum likelihood.

Figure 1 depicts the high-level structure of the proposed method, while Algorithm 1 gives the formal description. Initially, Algorithm 1 samples $n_1 + n_2$ architectures randomly and does low-fidelity evaluations of $n_1$ architectures and high-fidelity evaluations of $n_2$ architectures. After this warm-up, the architectures are selected cyclically by the UCB criteria (line 11) and evaluated via
Algorithm 1: MF-KD: A Multi-fidelity Neural Architecture Search Method with Knowledge Distillation

**Input:** \( X \) - search space of architectures (encodings in \( \mathbb{R}^d \)), \( n_1, n_2, E_1, E_2, N, T \) - total budget for the procedure, \( \beta \) - non-negative float (default 1.0, exploration/exploitation trade-off).

1. \( t = 0 \) // spent budget
2. Randomly sample \( n_1 \) architectures - \( A_1 \)
3. (I) Train architectures from \( A_1 \) for \( E_1 \) epochs with Knowledge Distillation (low-fidelity 1)
4. \( t + = \text{budget for (I)} \)
5. Randomly sample \( n_2 \) architectures - \( A_2 \)
6. (II) Train architectures from \( A_2 \) for \( E_2 \) epochs (low-fidelity 2)
7. \( t + = \text{budget for (II)} \)
8. Fit co-kriging fusion regression \( y^{(2)}(x) = \rho y^{(1)}(x) + \delta(x) \), where \( y^2(x) \) - predictions for low-fidelity 2 data, \( y^1(x) \) - predictions for low-fidelity 1 data, \( \delta(x) \) - discrepancy, \( y^{(2)}(x), y^{(1)}(x), \delta(x) \) are Gaussian Processes, \( y^{(1)} \) is independent of \( \delta, \rho \) - scaling factor (parameter).
9. while \( t < T \) do
10. Sample \( N \) random architectures - \( A \)
11. Select one architecture \( x^* \) from \( A \):
12. \( x^* = \arg\max_{x \in A} \left( \mathbb{E} \left[ y^{(2)}(x) \right] + \beta \text{Var} \left[ y^{(2)}(x) \right] \right) \)
13. (III) Train architecture \( x^* \) for \( E_2 \) epochs (low-fidelity 2)
14. \( t + = \text{budget for (III)} \)
15. Fit co-kriging fusion regression (with updated low-fidelity 2 data for \( x^* \))

**Return:** Architecture with the best validation score after \( E_2 \) epochs evaluated during the procedure.

The proposed model can be extended to more than two levels of fidelity using the schema proposed in [16]. Under the Markov assumptions on the covariance structures, each level of fidelity depends only on the previous one in the same fashion as high-fidelity depends on low-fidelity in [6].
Fig. 2: Top: macro-structure of the network. Bottom-left: example of stacked cells with various operations. Each cell is a directed acyclic graph. Each edge is associated with some operation. Bottom-right: the list of operations. Picture was redrawn from [8].

### 4 Experiments

#### 4.1 NAS benchmark

For the experiments, we used NAS-Bench-201 [8] benchmark. It contains 15,625 convolutional architectures trained on CIFAR-10, CIFAR-100 and ImageNet-16-120 (downsampled to 16×16 variant of ImageNet with 120 classes). Figure 2 shows macro- and micro-structure of the architectures. Each cell is stacked $N = 5$ times, number of output channels gradually increases from 16 to 64 from the first to the last layer. These architectures were trained with the following hyperparameters: 200 epochs, cosine annealing learning rate, momentum 0.9, initial learning rate 0.1, weight decay $5 \times 10^{-4}$, and augmentation (random crop, random flip). The benchmark provides thorough logs of training.

The test accuracy of top architectures from the NAS-Bench-201 is not state-of-the-art since the networks were trained for a not so many epochs with only basic augmentation techniques. Otherwise, training of 15,625 networks would be unfeasible.

**Encoding of the architectures.** Since the macro-structure is fixed, each architecture can be unequivocally described by it’s cell structure. We used concatenated one-hot encodings of operations associated with edges as encoding of the whole architecture.

#### 4.2 KD methods

In preliminary experiments with CIFAR-100 dataset (see Appendix) we tested various types of KD methods. We selected the NST method for the further ex-
Table 1: Kendall-tau correlation between low-fidelity and high-fidelity evaluations. Low-fidelity evaluations are done by training for 1 epoch.

| Loss       | Dataset          | CIFAR-10 | CIFAR-100 | ImageNet16-120 |
|------------|-----------------|----------|-----------|----------------|
| logistic loss | 0.17            | 0.06     | 0.21      |
| NST loss   | **0.47**        | **0.47** | **0.45**  |

We performed experiments with NAS-Bench-201 since it led to the highest correlation between low-fidelity and high-fidelity evaluations. In the NST loss, we used the polynomial kernel $k(x, y) = (x^T y + c)^b$ with $c = 0, b = 2$ and $\beta = 12.5$ in [3]. We used ResNet networks trained on the same datasets as teachers.

Unfortunately, calculating the gradient of the NST loss (3) adds significant overhead to the traditional logistic loss, training becomes $\approx 3$ times slower. To mitigate this issue, we calculated the NST loss approximately

$$
\sum_i \left( H(y_i, \sigma(z_i^S)) + \beta \tilde{L}_{MMD^2}(F_{i,T}, F_{i,S}) \right),
$$

with only a subset of feature maps $\tilde{C}_T \subset \{1, \ldots, C_T\}, \tilde{C}_S \subset \{1, \ldots, C_S\}^5$

$$
\tilde{L}_{MMD^2}(F^T, F^S) = \frac{1}{|\tilde{C}_T|^2} \sum_{i \in \tilde{C}_T} \sum_{i' \in \tilde{C}_T} k\left( \frac{f_{i,T}^i}{||f_{i,T}^i||_2}, \frac{f_{i,T}^{i'}}{||f_{i,T}^{i'}||_2} \right) + \frac{1}{|\tilde{C}_S|^2} \sum_{j \in \tilde{C}_S} \sum_{j' \in \tilde{C}_S} k\left( \frac{f_{j,S}^j}{||f_{j,S}^j||_2}, \frac{f_{j,S}^{j'}}{||f_{j,S}^{j'}||_2} \right) - \frac{2}{|\tilde{C}_T||\tilde{C}_S|} \sum_{i \in \tilde{C}_T} \sum_{j \in \tilde{C}_S} k\left( \frac{f_{i,T}^i}{||f_{i,T}^i||_2}, \frac{f_{j,S}^j}{||f_{j,S}^j||_2} \right).$$

After this optimization, training with the NST loss became only $\approx 1.5$ times slower$^6$. We didn’t perform a detailed study of this issue, and consider that selecting layers for doing knowledge distillation is an interesting topic for the further research.

Table 1 shows Kendall-tau rank correlations between low- and high-fidelity evaluations. Low-fidelity evaluations are done by training architectures for 1 epoch. We conclude that training with the NST loss significantly improves the correlation over the conventional logistic loss.

### 4.3 Multi-fidelity NAS

Finally, we tested the proposed MF-KD method (Algorithm 1) with the NAS-Bench-201 benchmark. We used parameters $E_1 = 1, E_2 = 12, n_1 = 100, n_2 = 5$: We used feature maps after 2 cells of N=5 stacked cells and each residual block (see Figure 2).

$^6$ Even more speed-up is possible by precomputing feature maps of the teacher network.
Table 2: Results of the MF-KD method. For each of the method, the accuracy of the best found architecture is shown. The search was performed under the same computational budget, averaged over 100 runs.

| Method          | CIFAR-10 | CIFAR-100 | ImageNet-16-120 |
|-----------------|----------|-----------|-----------------|
| DARTS-V2        | 54.30    | 15.61     | 16.32           |
| GDAS            | 93.51    | 70.61     | 41.84           |
| ENAS            | 54.30    | 15.61     | 16.32           |
| Reg. Evolution  | 93.92    | 71.84     | 45.54           |
| Random Search   | 93.70    | 71.04     | 44.57           |
| BOHB            | 93.61    | 70.85     | 44.42           |
| MF-KD           | 93.93    | 72.00     | 45.67           |

NAS methods were compared by the test accuracy of the best found architecture, averaged over 100 runs. NAS methods were allowed to use the equal computational budget – $12 \times 10^3$ seconds, same as in [8]. For all the methods except MF-KD we used the data from [8].

Table 2 presents the results. We conclude that the MF-KD method is the best performing one. Particularly, it found better architecture than the state-of-the-art multi-fidelity algorithm BOHB. The improvement over the second best method, Regularized Evolution, is significant with p-value $< 0.05$.

An alternative way to assess the NAS method’s quality is to compare results by the relative accuracy in the search space instead of the absolute accuracy. The MF-KD method found architectures having accuracy’s in top 0.3%, 0.2%, 0.5% within the search space for the datasets CIFAR-10, CIFAR-100, and ImageNet-16-120, respectively.

4.4 Ablation studies

The proposed method MF-KD has two contributions: bayesian multi-fidelity search and low-fidelity evaluations after training with the NST loss. We carry out ablation studies of these contributions:

- Search with a single fidelity: Gaussian Processes Regression (GPR) with high-fidelity evaluations only;
- Multi-fidelity search, where low-fidelity evaluations are training with the conventional logistic loss for a few epochs;

---

7 The co-kriging regression in the Algorithm 1 is fitted to the validation accuracy, while the methods are compared by the test accuracy of the best architectures. Model selection based on validation accuracy while estimating performance by test accuracy is a common pattern for AutoML/NAS algorithms performed to avoid overfitting.
Table 3: Ablation studies of the MF-KD method. For each of the method, the accuracy of the best found architecture is shown. The search was performed under the same computational budget, averaged over 100 runs.

| Method                  | Accuracy, % |
|-------------------------|-------------|
|                         | CIFAR-10 | CIFAR-100 | ImageNet-16-120 |
| ResNet                  | 93.97     | 70.86     | 44.63           |
| Single fidelity (GPR)   | 93.78     | 71.44     | 45.44           |
| Multi-fidelity (no KD)  | 93.93     | 71.83     | 45.41           |
| MF-KD                   | 93.93     | 72.00     | 45.67           |

Table 3 shows the results: both of the contributions improve the algorithm’s performance for more CIFAR-100 and ImageNet-16-120 datasets. For simpler CIFAR-10 this not the case. Also, for CIFAR-100 and ImageNet-16-120 the proposed method found the architecture better than the teacher, ResNet.

5 Conclusion

In this work, we have proposed the new MF-KD method tailored to neural architecture search. By doing experiments, we have proved that the MF-KD method is efficient. It leads to a better architecture selection than several state-of-the-art baselines given the same computational budget. Also it outperforms state-of-the-art multi-fidelity method BOHB. We validated our contributions on the NAS-Bench-201 benchmark, including CIFAR-10, CIFAR-100 and ImageNet-16-120 datasets.

Our research gives an interesting insight into knowledge distillation methods themselves. While these methods are typically compared by a performance of compact student networks trained with the KD loss, we apply the KD loss to improve architecture selection after training for a few epochs.

Our work satisfies the best practices for scientific research on NAS [24], see Appendix A.

References

1. Adam, G., Lorraine, J.: Understanding neural architecture search techniques. arXiv preprint arXiv:1904.00438 (2019)
2. Ahn, S., Hu, S.X., Damianou, A., Lawrence, N.D., Dai, Z.: Variational information distillation for knowledge transfer. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition. pp. 9163–9171 (2019)
3. Bender, G.: Understanding and simplifying one-shot architecture search (2019)
4. Cai, H., Zhu, L., Han, S.: Proxylessnas: Direct neural architecture search on target task and hardware. arXiv preprint arXiv:1812.00332 (2018)
5. Chen, X., Xie, L., Wu, J., Tian, Q.: Progressive differentiable architecture search: Bridging the depth gap between search and evaluation. In: Proceedings of the IEEE International Conference on Computer Vision. pp. 1294–1303 (2019)
6. Chrbašec, P., Loshchilov, I., Hutter, F.: A downsampled variant of imagenet as an alternative to the cifar datasets. arXiv preprint arXiv:1707.08819 (2017)
7. Dong, X., Yang, Y.: Searching for a robust neural architecture in four gpus hours. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition. pp. 1761–1770 (2019)
8. Dong, X., Yang, Y.: Nas-bench-201: Extending the scope of reproducible neural architecture search. arXiv preprint arXiv:2001.00326 (2020)
9. Elsken, T., Metzen, J.H., Hutter, F.: Efficient multi-objective neural architecture search via lamarckian evolution. arXiv preprint arXiv:1804.00081 (2018)
10. Guo, Z., Zhang, X., Mu, H., Heng, W., Liu, Z., Wei, Y., Sun, J.: Single path one-shot neural architecture search with uniform sampling. arXiv preprint arXiv:1904.00420 (2019)
11. Hinton, G., Vinyals, O., Dean, J.: Distilling the knowledge in a neural network. arXiv preprint arXiv:1503.02531 (2015)
12. Huang, Z., Wang, N.: Like what you like: Knowledge distill via neuron selectivity transfer. arXiv preprint arXiv:1707.01219 (2017)
13. Kandasamy, K., Dasarathy, G., Oliva, J., Schneider, J., Poczos, B.: Multi-fidelity gaussian process bandit optimisation. Journal of Artificial Intelligence Research 66, 151–196 (2019)
14. Kandasamy, K., Neiswanger, W., Schneider, J., Poczos, B., Xing, E.P.: Neural architecture search with bayesian optimisation and optimal transport. In: Advances in Neural Information Processing Systems. pp. 2016–2025 (2018)
15. Kang, M., Mun, J., Han, B.: Towards oracle knowledge distillation with neural architecture search. AAAI (2020)
16. Kennedy, M.C., O’Hagan, A.: Predicting the output from a complex computer code when fast approximations are available. Biometrika 87(1), 1–13 (2000)
17. Kim, Y., Rush, A.M.: Sequence-level knowledge distillation. arXiv preprint arXiv:1606.07947 (2016)
18. Klein, A., Falkner, S., Bartels, S., Hennig, P., Hutter, F.: Fast bayesian optimization of machine learning hyperparameters on large datasets. arXiv preprint arXiv:1605.07079 (2016)
19. Klyuchnikov, N., Mottin, D., Koutrakis, G., Müller, E., Karras, P.: Figuring out the user in a few steps: Bayesian multifidelity active search with cokriging. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining. pp. 686–695 (2019)
20. Krizhevsky, A., Hinton, G., et al.: Learning multiple layers of features from tiny images (2009)
21. Li, C., Peng, J., Yuan, L., Wang, G., Liang, X., Lin, L., Chang, X.: Blockwisely supervised neural architecture search with knowledge distillation. CVPR (2020)
22. Li, L., Talwalkar, A.: Random search and reproducibility for neural architecture search. arXiv preprint arXiv:1902.07638 (2019)
23. Liang, H., Zhang, S., Sun, J., He, X., Huang, W., Zhuang, K., Li, Z.: Darts+: Improved differentiable architecture search with early stopping. arXiv preprint arXiv:1909.06035 (2019)
24. Lindauer, M., Hutter, F.: Best practices for scientific research on neural architecture search. arXiv preprint arXiv:1909.02453 (2019)
25. Liu, H., Simonyan, K., Yang, Y.: Darts: Differentiable architecture search. arXiv preprint arXiv:1806.09055 (2018)
26. Liu, Y., Jia, X., Tan, M., Vemulapalli, R., Zhu, Y., Green, B., Wang, X.: Search to distill: Pearls are everywhere but not the eyes. CVPR (2020)
27. Ma, N., Zhang, X., Zheng, H.T., Sun, J.: Shufflenet v2: Practical guidelines for efficient cnn architecture design. In: Proceedings of the European Conference on Computer Vision (ECCV). pp. 116–131 (2018)
28. Passalis, N., Tefas, A.: Learning deep representations with probabilistic knowledge transfer. In: Proceedings of the European Conference on Computer Vision (ECCV). pp. 268–284 (2018)
29. Pedregosa, F.: Hyperparameter optimization with approximate gradient. arXiv preprint arXiv:1602.02355 (2016)
30. Peng, B., Jin, X., Liu, J., Li, D., Wu, Y., Liu, Y., Zhou, S., Zhang, Z.: Correlation congruence for knowledge distillation. In: Proceedings of the IEEE International Conference on Computer Vision. pp. 5007–5016 (2019)
31. Pham, H., Guan, M.Y., Zoph, B., Le, Q.V., Dean, J.: Efficient neural architecture search via parameter sharing. arXiv preprint arXiv:1802.03268 (2018)
32. Real, E., Aggarwal, A., Huang, Y., Le, Q.V.: Regularized evolution for image classifier architecture search. In: Proceedings of the aaai conference on artificial intelligence. vol. 33, pp. 4780–4789 (2019)
33. Romero, A., Ballas, N., Kahou, S.E., Chassang, A., Gatta, C., Bengio, Y.: Fitnets: Hints for thin deep nets. arXiv preprint arXiv:1412.6550 (2014)
34. Rusu, A.A., Colmenarejo, S.G., Gulcehre, C., Desjardins, G., Kirkpatrick, J., Pascanu, R., Mnih, V., Kavukcuoglu, K., Hadsell, R.: Policy distillation. arXiv preprint arXiv:1511.06295 (2015)
35. Sandler, M., Howard, A., Zhu, M., Zhmoginov, A., Chen, L.C.: Mobilenetv2: Inverted residuals and linear bottlenecks. In: Proceedings of the IEEE conference on computer vision and pattern recognition. pp. 4510–4520 (2018)
36. Shi, H., Pi, R., Xu, H., Li, Z., Kwok, J.T., Zhang, T.: Multi-objective neural architecture search via predictive network performance optimization. arXiv preprint arXiv:1911.09336 (2019)
37. Song, J., Chen, Y., Yue, Y.: A general framework for multi-fidelity bayesian optimization with gaussian processes. arXiv preprint arXiv:1811.00755 (2018)
38. Tian, Y., Krishnan, D., Isola, P.: Contrastive representation distillation. arXiv preprint arXiv:1910.10699 (2019)
39. Tung, F., Mori, G.: Similarity-preserving knowledge distillation. In: Proceedings of the IEEE International Conference on Computer Vision. pp. 1365–1374 (2019)
40. White, C., Neiswanger, W., Savani, Y.: Bananas: Bayesian optimization with neural architectures for neural architecture search. arXiv preprint arXiv:1910.11858 (2019)
41. Williams, C.K., Rasmussen, C.E.: Gaussian processes for machine learning, vol. 2. MIT press Cambridge, MA (2006)
42. Xu, Y., Xie, L., Zhang, X., Chen, X., Qi, G.J., Tian, Q., Xiong, H.: Pc-darts: Partial channel connections for memory-efficient differentiable architecture search. arXiv preprint arXiv:1907.05737 (2019)
43. Yang, A., Esperança, P.M., Carlucci, F.M.: Nas evaluation is frustratingly hard. arXiv preprint arXiv:1912.12522 (2019)
44. Ying, C., Klein, A., Real, E., Christiansen, E., Murphy, K., Hutter, F.: Nas-bench-101: Towards reproducible neural architecture search. arXiv preprint arXiv:1902.09635 (2019)
45. Zagoruyko, S., Komodakis, N.: Paying more attention to attention: Improving the performance of convolutional neural networks via attention transfer. arXiv preprint arXiv:1612.03928 (2016)
The best practices of NAS research are the following [24]:

1. Release Code for the Training Pipeline(s) you use;
2. Release Code for Your NAS Method;
3. Don’t Wait Until You’ve Cleaned up the Code; That Time May Never Come;
4. Use the Same NAS Benchmarks, not Just the Same Datasets;
5. Run Ablation Studies;
6. Use the Same Evaluation Protocol for the Methods Being Compared;
7. Compare Performance over Time;
8. Compare Against Random Sampling and Random Search;
9. Validate The Results Several Times;
10. Use Tabular or Surrogate Benchmarks If Possible;
11. Control Confounding Factors;
12. Report the Use of Hyperparameter Optimization;
13. Report the Time for the Entire End-to-End NAS Method;
14. Report All the Details of Your Experimental Setup.

We released all the code (1, 2, 3). We carried out experiments on the public tabular benchmark (4, 10). We did ablation studies in Section 4.4 (5). Since we used tabular benchmark (6) is satisfied. For multi-fidelity optimization, we made comparisons over time (7). We compared against random search (8). Experimental results are averaged over many runs (9). We did our best to control confounding factors (11). Hyperparameter optimization (12) is described in Appendix B. We did our best to report all the details about the experimental setup (14). We also discuss computational performance in the Section 4.2.

B Comparison of KD methods

Initially, we evaluated various KD methods on two small search spaces: 100 modifications of MobileNetV2 [35] and 300 modifications of ShuffleNetV2 [27] architectures.

These architectures share the same pattern – particular human-designed blocks are repeated certain number of times while channels count increase from input to output. To create search spaces, we randomly modified repetitions and channels counts while preserving the increasing pattern of channels from input.
Table 4: Correlation between high-fidelity and low-fidelity evaluations.

| Part | Pearson corr. |
|------|---------------|
|      | no KD | orig. | KD | AT | NST | SS | VID | PKT | CRD | Hint | CC |
| MobileNetV2 search space |
| 1/27 | 0.11  | 0.34  | 0.57 | 0.42 | 0.35 | -0.03 | 0.35 | 0.18 | 0.19 | 0.16 |
| 1/9  | 0.46  | 0.61  | 0.61 | 0.60 | 0.53 | 0.07  | 0.47 | 0.44 | 0.48 | 0.45 |
| 1/3  | 0.86  | 0.92  | 0.74 | 0.81 | 0.79 | -0.21 | 0.41 | 0.85 | 0.84 | 0.90 |
| ShuffleNetV2 search space |
| 1/27 | 0.48  | 0.54  | 0.43 | 0.61 | 0.45 | 0.45  | 0.44 | 0.43 | 0.47 | 0.46 |
| 1/9  | 0.64  | 0.81  | 0.57 | 0.74 | 0.61 | 0.60  | 0.60 | 0.30 | 0.64 | 0.58 |
| 1/3  | **0.92** | 0.91  | 0.72 | **0.93** | 0.91 | 0.92  | 0.76 | 0.88 | 0.91 | **0.92** |

To output. These numbers – repetitions and channels count – were used as architectures’ features. The dimensionality of the MobileNetV2 search space is 16, the ShuffleNetV2 search space – 7. To avoid too small and too large architectures, we left only ones having a number of parameters in the range \( (1/3P, 3P) \), where \( P \) is the number of the parameters of the original MobileNetV2 and ShuffleNetV2 respectively. We have trained all the architectures on the full CIFAR-100 [20] dataset, and its \( 1/27, 1/9, 1/3 \) random but fixed subsets (instead of few epochs). Various loss functions were tested: logistic loss (no KD), knowledge distillation methods: original KD [11], Hint [33], AT [45], SP [39], CC [30], VID [2], PKT [28], NST [12], CRD [38]. The hyperparameters of training were: 100 epochs, momentum 0.9, cosine annealing learning rate, initial learning rate 0.1, weight decay \( 5 \times 10^{-4} \), batch size 128 with random cropping and horizontal flipping. The hardware was GeForce GTX 1080 Ti. Teachers in search spaces were original MobileNetV2 and ShuffleNetV2 architectures trained on the same dataset with the same hyperparameters.

### Hyperparameters tuning

We have tuned hyperparameters of KD methods by doing low-fidelity evaluations of 20 random architectures with training on a \( 1/9 \) part of the CIFAR-100 dataset. Then we have selected the best combination by the highest correlation with high-fidelity evaluations, see Table 5. The same hyperparameters were used for the NST loss for main experiments with NAS-Bench-201 benchmark (Section 4). Table 4 shows correlation between high-fidelity and low-fidelity evaluations for the best hyperparameters. We conclude that the AT and NST loss (AT loss is the particular case of NST loss) perform the best for the evaluation by training on \( 1/27 \) of the dataset.

### C Additional experiments with ImageNet

We did low-fidelity evaluations of all the architectures from the MobileNetV2 search space by training on \( 1/27 \) part of the ImageNet dataset. For low-fidelity
Table 5: Optimal hyperparameters of KD methods

| KD method                                               | MobileNetV2 search space | ShuffleNetV2 search space |
|---------------------------------------------------------|--------------------------|---------------------------|
| Distilling the knowledge in a neural network [11] (KD)   | τ = 32, λ = 1            |                           |
| Fitnets: Hints for thin deep nets [33] (Hint)           | β = 100                  |                           |
| Attention Transfer (AT) [45]                           | β = 10³, β = 4 × 10³     |                           |
| Similarity-Preserving Knowledge Distillation (SP) [39]  | β = 750, β = 90          |                           |
| Correlation Congruence (CC) [30]                        | β = 0.5 × 10⁻²           |                           |
| Variational information distillation                    | β = 0.01, β = 0.25       |                           |
| for knowledge transfer (VID)                            |                          |                           |
| Learning deep representations                          | β = 48 × 10⁴             |                           |
| with probabilistic knowledge transfer (PKT) [28]        |                          |                           |
| Like what you like:                                    | β = 12.5, β = 200        |                           |
| Knowledge distill via neuron select. transfer (NST) [12]|                          |                           |
| Contrastive Representation Distillation (CRD) [38]      | τ = 0.2, β = 0.5, τ = 0.05, β = 1 |   |

evaluations, we trained for 100 epochs and other hyperparameters were the same as for low-fidelity evaluations on CIFAR-100.

For high-fidelity evaluations, we used the following hyperparameters: 150 epochs with momentum 0.9, cosine annealing learning rate, initial learning rate 0.05, weight decay 4 × 10⁻⁵, batch size 128, the augmentation included random cropping and horizontal flipping.

Additionally, we did high-fidelity and low-fidelity evaluations of 10 random architectures and calculated Kendall-tau correlation between high- and low-fidelity evaluations. For conventional logistic loss, it turned out 0.42, while for the original KD loss 0.73. The increase in the correlation confirms our conclusions.