FP-NAS: Fast Probabilistic Neural Architecture Search

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Abstract

Differential Neural Architecture Search (NAS) requires all layer choices to be held in memory simultaneously; this limits the size of both search space and final architecture. In contrast, Probabilistic NAS, such as PARSEC, learns a distribution over high-performing architectures, and uses only as much memory as needed to train a single model. Nevertheless, it needs to sample many architectures, making it computationally expensive for searching in an extensive space. To solve these problems, we propose a sampling method adaptive to the distribution entropy, drawing more samples to encourage explorations at the beginning, and reducing samples as learning proceeds. Furthermore, to search fast in the multi-variate space, we propose a coarse-to-fine strategy by using a factorized distribution at the beginning which can reduce the number of architecture parameters by over an order of magnitude. We call this method Fast Probabilistic NAS (FP-NAS). Compared with PARSEC, it can sample 64% fewer architectures and search 2.1 × faster. Compared with FBNetV2, FP-NAS is 1.9 × - 3.6 × faster, and the searched models outperform FBNetV2 models on ImageNet. FP-NAS allows us to expand the giant FBNetV2 space to be wider (i.e. larger channel choices) and deeper (i.e. more blocks), while adding Split-Attention block and enabling the search over the number of splits. When searching a model of size 0.4G FLOPS, FP-NAS is 132× faster than EfficientNet, and the searched FP-NAS-L0 model outperforms EfficientNet-B0 by 0.6% accuracy. Without using any architecture surrogate or scaling tricks, we directly search large models up to 1.0G FLOPS. Our FP-NAS-L2 model with simple distillation outperforms BigNAS-XL with advanced inplace distillation by 0.7% accuracy with less FLOPS.

1. Introduction

Designing efficient architectures for visual recognition requires extensive exploration in the search space; doing this by hand takes substantial human effort and computational resources. Since the introduction of AlexNet [18], hand-crafted models like ResNet [10], Densenet [14] and InceptionV4 [28], have become increasingly deep with more complex connectivity. Exploring this space manually is difficult and time-consuming. Neural Architecture Search (NAS) aims to automate the architecture design process. However, early approaches based on evolution or reinforcement learning take hundreds or thousands of GPU days just for CIFAR10 or Imagenet target datasets [42, 43, 31, 25].

Recently, differentiable neural architecture search (DNAS) [20] relaxed the discrete representation of architectures to a continuous space, enabling efficient search with gradient descent. This comes at a price: DNAS instantiates all layer choices in memory, and computes all feature maps. Therefore, its memory footprint increases linearly with the number of layer choices, and greatly limits the size of both search space and final architecture. PARSEC [4] presents a probabilistic version of DNAS which samples individual architectures from a distribution on search space. PARSEC’s sampling strategy uses much less memory, but it samples a large number of architectures to fully explore the space, which significantly increases computational cost. Here we pose the following question: *Can we reduce PARSEC’s compute cost and maintain a small memory footprint to support the fast search of both small and large models?*

In this work, we accelerate PARSEC by proposing two novel techniques. First, we replace the fixed architecture sampling with a dynamic sampling adaptive to the entropy of architecture distribution. In particular, we sample more architectures in the early stage to encourage exploration, and fewer later, as the distribution concentrates on a smaller set of promising architectures. Furthermore, in multi-variate space where several variables (e.g. block type, feature channel, expansion ratio) are searched over, we propose a coarse-to-fine search strategy. In the beginning stage, we adopt a factorized distribution representation to search at a coarse-grained granularity, which uses much fewer architecture parameters and makes the learning much faster. In the following stage, we seamlessly convert the factorized distribution into the joint distribution to support fine-grained search.

When searching in the FBNetV2 space [33], FP-NAS samples 64% fewer architectures and searches 2.1 × faster compared with the PARSEC method. Compared with FBNetV2, FP-NAS is 3.6× faster, and the searched models outperform FBNetV2 models on ImageNet. To fur-
We also use notation (+ distill) which increases the space size by obtained via direct search. To our knowledge, this is the largest architecture search on a subset of ImageNet, uses 9970 single crop. Moreover, our method also discovers more superior FP-NAS-of EfficientNet-B0 × 0.4G target FLOPS, FP-NAS only uses 28.7× higher accuracy on ImageNet. The largest model we searched is FP-NAS-L2, which uses nearly 1G FLOPS, outperform EfficientNet-B2 by 0.3% top-1 accuracy, while the search cost is much lower.

We expand FBNetV2 search space by replacing Squeeze-Excite module [13] with searchable Split-Attention (SA) module [39]. We demonstrate uniformly inserting SA modules to the model with a fixed number of splits, as done in hand-crafted ResNeSt [39] models, is sub-optimal, and models with searched SA modules are more competitive.

2. Related Work

Hand-Crafted Models. The conventional way of building ConvNet is to design repeatable building blocks, and stack them to form deep models, including ResNet [10, 35], DenseNet [14], and Inception [30, 29, 28]. Meanwhile, manually designing compact mobile models has also attracted lots of interest due the prevalence of mobile devices. Mobile models uses more compute-efficient blocks, such as inverted residual block [27] and shuffling layers [40, 21]. However, recent models discovered by neural architecture search have surpassed hand-crafted models in various tasks [9, 32, 1, 24].

Non-Differentiable Neural Architecture Search. Early NAS methods are based on either reinforcement learning (RL) [31] or evolution [26]. In the pioneering work [42], a RNN controller is adopted to sample architectures, which are trained to obtain accuracy as the reward signal for updating the controller. It requires to train tens of thousands of architectures, which is computationally prohibitive. Similarly, in NASNet [43], it takes 2,000 GPU days to search architectures for CIFAR10 and ImageNet. In the AmoebaNet [25], which is based on evolution, the search algorithm iteratively evaluates a small number of child architectures evolved from the best-performing architectures in the population to speed up the search, but still requires to train thousands of individual architectures. Recently, EfficientNet [32] built big models by scaling up the small ones from RL-based search [31].

An adaptive sampling method for fast probabilistic NAS, which can sample 60% fewer architectures and accelerate the search in FBNetV2 space by 1.8×.

A coarse-to-fine search method by adopting a factorized distribution representation with much fewer architecture parameters in the early coarse-grained search stage. It can further accelerate the overall search by 1.2×.

For searching small models, comparing with FBNetV2, FP-NAS is not only 3.6× faster, but also discovers models with substantially better accuracy-to-complexity trade-off.

For searching large models, compared with EfficientNet, when searching models of 0.4G FLOPS, FP-NAS is not only 132× faster, but also discovers a model with 0.6% higher accuracy on ImageNet. The largest model we searched is FP-NAS-L2, which uses nearly 1G FLOPS, outperform EfficientNet-B2 by 0.3% top-1 accuracy, while the search cost is much lower.

To summarize, this work makes the contributions below:

- For searching small models, comparing with FBNetV2, FP-NAS is not only 3.6× faster, but also discovers models with substantially better accuracy-to-complexity trade-off.
- For searching large models, compared with EfficientNet, when searching models of 0.4G FLOPS, FP-NAS is not only 132× faster, but also discovers a model with 0.6% higher accuracy on ImageNet. The largest model we searched is FP-NAS-L2, which uses nearly 1G FLOPS, outperform EfficientNet-B2 by 0.3% top-1 accuracy, while the search cost is much lower.
- For searching small models, comparing with FBNetV2, FP-NAS is not only 3.6× faster, but also discovers models with substantially better accuracy-to-complexity trade-off.
- For searching large models, compared with EfficientNet, when searching models of 0.4G FLOPS, FP-NAS is not only 132× faster, but also discovers a model with 0.6% higher accuracy on ImageNet. The largest model we searched is FP-NAS-L2, which uses nearly 1G FLOPS, outperform EfficientNet-B2 by 0.3% top-1 accuracy, while the search cost is much lower.
jointly along the depth, width and input resolution. BigNAS [38] trains a single-stage model with inplace distillation, and induce child models of different sizes without retraining or fine-tuning. In this work, with the proposed fast probabilistic NAS method, we show directly searched big architectures without any scaling trick can achieve a better accuracy-to-complexity trade-off.

**Differentiable Neural Architecture Search.** DARTS [20] relaxes the discrete search space to be continuous, and optimizes the architecture by gradient descent. While being much faster, it requires to instantiate all layer choices in the memory, making it difficult to directly search big architectures in large space. Therefore, DARTS needs to use a shallow version of model at search time to serve as the surrogate, and repeats the searched cells many more times at evaluation time to build larger models.

Following works improve DARTS by path pruning to reduce memory footprint as in ProxylessNAS [2], more fine-grained search space [22], hierarchical search space [19], better optimizer [23], better architecture sampler [5], being platform-aware [34, 7], and searching over channels and input resolution in a memory efficient manner [33]. In GDAS [8] paper, a differentiable sampler based on Gumbel-Max trick [16] is proposed to only sample one architecture at a time. This reduces the memory usage but the searched architectures have performance inferior to those searched by evolution-based methods [25]. PARSEC [4] proposes a sampling-based method to learn a probability distribution over architectures, and is also memory-efficient. However, to achieve good search results, it needs to constantly sample a large number of architectures, which is computationally expensive. In this work, we propose to adaptively reduce the architecture samples based on entropy of architecture distribution, substantially reduce the search time, and enable the search of bigger architectures.

For searching mobile models, differentiable NAS methods are adapted to be hardware-aware, considering model cost, such as FLOPS, memory, latency on specific hardware [34, 33, 7, 31, 12]. In this work, we adopt a hinge-linear penalty on the model FLOPS to constrain the computational cost and support the search of models with target FLOPS.

### 3. Fast Probabilistic NAS

#### 3.1. Background

Our method extends PARSEC [4] (a probabilistic NAS), which we briefly review here. In DNAS [20], for each layer \( l \) we have a set of candidate operations \( O \); each operation \( o(\cdot) \) can be applied to input feature \( x_l \). Discrete choice is relaxed to a weighted sum of candidate operations:

\[
x_l^{t+1} = \sum_{o \in O} \frac{\exp(o_{\alpha}^t)}{\sum_{o' \in O} \exp(o_{\alpha}^t)} o(x_l)
\]

where \( \{o_{\alpha}^t\}_{o \in O} \) denotes the architecture parameters at layer \( l \).

An architecture \( A \) is uniquely defined by the individual choices at \( L \) layers \( A = (A^1, ..., A^L) \). In PARSEC, a prior distribution \( \mathcal{P}(A | \alpha) \) on the choices of layer operation is introduced, where architecture parameters \( \alpha \) denote the probabilities of choosing different operations. Individual architectures can be represented as discrete choices of \( \{A^l\} \) and sampled from \( \mathcal{P}(A | \alpha) \). Therefore, architecture search is transformed into learning the distribution \( \mathcal{P}(A | \alpha) \) under certain supervision. For simplicity, we first assume the choices at different layers are independent to each other, and the probability of sampling an architecture \( A \) is shown below.

\[
\mathcal{P}(A | \alpha) = \prod_l \mathcal{P}(A^l | \alpha^l)
\]

For image classification where we have images \( X \) and labels \( y \), probabilistic NAS can be formulated as optimizing the continuous architecture parameters \( \alpha \) via an empirical Bayes Monte Carlo procedure [3]

\[
P(y|X, \omega, \alpha) = \int P(y|X, \omega, A) \mathcal{P}(A | \alpha) dA \\
\approx \frac{1}{K} \sum_k P(y|X, \omega, A_k)
\]

where \( \omega \) denotes the model weights. The continuous integral of data likelihood is approximated by sampling architectures and averaging the data likelihoods from them. We can jointly optimize architecture parameters \( \alpha \) and model weights \( \omega \) by estimating gradients \( \nabla_{\alpha} \log P(y|X, \omega, \alpha) \) and \( \nabla_{\omega} \log P(y|X, \omega, \alpha) \) through the sampled architectures.

To reduce over-fitting, separate training- and validation set are used to compute gradients w.r.t \( \alpha \) and \( \omega \), respectively. The probabilistic NAS proceeds in an iterative way. In each iteration, \( K \) architecture samples \( \{A_k\}_{k=1}^K \) are drawn from \( \mathcal{P}(A | \alpha) \).

For sampled architectures, gradients w.r.t \( \alpha \) and \( \omega \) in sampled operations are computed on a batch of training data. The detailed derivation of the gradients as well as the pseudo-algorithm can be seen in the supplement.

#### 3.2. Adaptive Architecture Sampling

In PARSEC [4], a fixed number of architectures are sampled during the entire search to estimate the gradients. For example, to search cell structures in the DARTS [20] space on CIFAR10 (a relatively small search space), the number of samples is held fixed at 16. Such choice is ad-hoc and could be suboptimal for searching in spaces of different size. In the beginning of the search where the architecture distribution \( \mathcal{P}(A | \alpha) \) is flat, a larger number of samples are needed to approximate the gradients. As the search
proceeds, the distribution concentrates mass on a small set of candidates. In such case, we can reduce the search computation by drawing fewer samples.

Formally, we propose a simple yet effective sampling method adaptive to the learning of architecture distribution. During the search, we adjust the size of architecture samples \( K \) to be proportional to the entropy of \( P(A|\alpha) \). Early in the search, entropy is high, encouraging more exploration. Later, entropy decreases as a subset of candidate operations are deemed to be more promising, and the sampling can be more biased towards them. Specifically, we set

\[
K = \lambda \cdot H(P(A|\alpha))
\]

where \( H \) denotes the distribution entropy, and \( \lambda \) a predefined scaling factor. In Section 5.2, we show adaptive sampling can greatly reduce the search time without degrading the searched model. The choice of \( \lambda \) is discussed in Section 5.2.1.

3.3. Coarse-to-Fine Search in Multi-Variate Space

The search space of each layer operation \( A_l \) can include multiple search variables, such as convolution kernel size, nonlinearity and feature channel. In such multi-variate space, when we use a vanilla joint distribution (JD) representation, the number of architecture parameters is a product of cardinalities of individual variables, which grows rapidly as more variables are added. For example, the search space used later in this work (See Table 1 and 2) has 5 variables, including kernel size, nonlinearity, Squeeze-Excite, expansion rate in MobileNetV3 [12] and channel. When their individual cardinalities are 3, 2, 2, 6, and 10 respectively, the JD uses \( \text{prod}([3, 2, 2, 6, 10]) = 720 \) parameters. We can factorize the large JD, and obtain a more compact representation using multiple small distributions. For the 5-dimensional search space above, we use 5 small distributions, and the total architecture parameters can be dramatically reduced to \( \text{sum}([3, 2, 2, 6, 10]) = 23 \), which is over \( 31 \times \) less.

Formally, in a search space of layer operation \( A_l \) with \( M \) search variables, each layer can be represented as a \( M \)-tuple \( A_l = (A_{l1}, ..., A_{lM}) \). We adopt a factorized distribution (FD) for the layer operation below.

\[
P(A_l|\alpha_l) = P(\{A_{ml}\}_{m=1}^{M}|\alpha_{ml}, m=1)
\]

\[
= \prod_{m=1}^{M} P(A_{ml}|\alpha_{ml}) \quad \text{where} \quad A_{ml} \in D_{ml}^l
\]

Here, \( D_{ml}^l \) denotes the set of choices for variable \( A_{ml} \). Compared with JD, FD greatly reduces the total architecture parameters from \( \prod_{m} |D_{ml}^l| \) to \( \sum_{m} |D_{ml}^l| \), which often leads to more than an order of magnitude reduction in practice, and can greatly accelerate the search. However, FD ignores the correlation between search variables, and can only support coarse-grained search. For example, the search of expansion rate and channel is likely to be correlated since the inner channel within the MBCConv block as in MobileNetV3 [12] is a product of expansion rate and channel. A large expansion rate might be more preferred when the channel is not high, but can be less preferred when the channel is already high because it can introduce an excessive amount of FLOPS but does not improve the classification accuracy.

To support fast search, we propose a coarse-to-fine search method by using a schedule of mixed distributions which starts the search with FD for a number of epochs, and later converts FD to the JD for the following epochs. As shown in Section 5.3, the coarse-to-fine search can accelerate the search without compromising the performance of the searched model.

3.4. Architecture Cost Aware Search

Without any constraint on the architecture cost (e.g. FLOPS, parameters or latency), the search tends to favor big architectures, which are more likely to fit training data better but might not be suitable for efficiency-sensitive applications. To search architectures with a target cost in mind, we adopt a hinge loss, which penalizes architectures when they use more than the target cost. We use FLOPS as the model cost in this work, but other choices, such as latency, can also be used. Our full cost-aware loss consists of the data likelihood and the model cost.

\[
\mathcal{L}(\omega, \alpha) = -\log P(y|X, \omega, \alpha) + \beta \log C(\alpha)
\]

\[
C(\alpha) = \int C(A)P(A|\alpha)d\alpha \approx \frac{1}{K} \sum_{k} C(A_k)
\]

where the hinge cost for a sampled architecture is \( C(A_k) = \max(0, \text{FLOPS}(A_k) - 1) \), \( \beta \) denotes the coefficient of architecture cost, and \( C(\alpha) \) the expected architecture cost, which can be estimated by averaging the costs of sampled architectures. The computation of gradient w.r.t \( \alpha \) is shown in Eq.(7).

\[
\nabla_\alpha \mathcal{L}(\omega, \alpha) \approx \sum_{k=1}^{K} m_k \nabla_\alpha - \log P(A_k|\alpha)
\]

where \( m_k = \frac{P(y|X, \omega, A_k)}{\sum_{i} P(y, \omega, A_i)} - \beta \frac{C(A_k)}{\sum_{i} C(A_i)} \), and denotes cost-aware architecture important weights. Intuitively, architecture parameters \( \alpha \) are updated to bias towards those architectures which both achieve high data likelihood on the validation data and use low FLOPS. At the end of the search, we select the most probable one in the learned distribution as the final architecture.

4. Search Spaces

We consider 4 difference spaces below to search models.
**Table 1: FBNetV2-F macro architecture.** Each row represents a block group. MBConv denotes the inverted residual block in MobileNetV2 [27]. Expansion and Channel denote expansion rate and the output channel of the block. Their search range is denoted as \((\text{min, max, step})\). Repeat denotes the repeating times of the block, and \textit{stride} means the stride of first one among them.

| Max Input \((S^2 \times C)\) | Operator | Expansion | Channel | Repeat | Stride |
|-------------------------------|----------|-----------|---------|--------|--------|
| \(224^2 \times 3\) | conv \(3 \times 3\) | 1         | 16      | 1      | 2      |
| \(112^2 \times 16\) | MBConv \((0.75, 4.5, 0.75)\) | 1         | \((12, 16, 4)\) | 1      | 1      |
| \(56^2 \times 24\) | MBConv \((0.75, 4.5, 0.75)\) | \((16, 24, 4)\) | 2      | 2      |
| \(56^2 \times 24\) | MBConv \((0.75, 4.5, 0.75)\) | \((16, 24, 4)\) | 2      | 2      |
| \(28^2 \times 40\) | MBConv \((0.75, 4.5, 0.75)\) | \((16, 40, 8)\) | 2      | 2      |
| \(28^2 \times 40\) | MBConv \((0.75, 4.5, 0.75)\) | \((16, 40, 8)\) | 2      | 2      |
| \(14^2 \times 80\) | MBConv \((0.75, 4.5, 0.75)\) | \((48, 80, 8)\) | 1      | 2      |
| \(14^2 \times 80\) | MBConv \((0.75, 4.5, 0.75)\) | \((72, 112, 8)\) | 3      | 1      |
| \(14^2 \times 112\) | MBConv \((0.75, 4.5, 0.75)\) | \((112, 184, 8)\) | 1      | 2      |
| \(7^2 \times 184\) | MBConv \((0.75, 4.5, 0.75)\) | \((112, 184, 8)\) | 3      | 1      |
| \(7^2 \times 184\) | conv \(1 \times 1\) | -         | \(1984\) | 1      |
| \(7^2 \times 1984\) | avgpool | -        | 1000    | 1      |

**Figure 2: MBConv block with searchable Split-Attention module.**

**FBNetV2-F space [33].** We conduct most ablation studies in this space, which is defined by the macro-architecture in Table 1, and the micro-architecture in the 1st row of Table 2. It has multiple search variables, including convolution kernel size, nonlinearity type, the use of Squeeze-Excite block [13], block expansion rate, and block feature channel, and contains \(6 \times 10^{25}\) different architectures.

**FBNetV2-F-Fine space.** The difference from FBNetV2-F space is each MBConv block is allowed to have different micro-architecture. FBNetV2-F-Fine contains \(1 \times 10^{45}\) architectures, which is \(10^{13}\) larger than FBNetV2-F, and can be viewed as a fine-grained version of FBNetV2-F space.

**FBNetV2-F++ space.** To demonstrate the search efficiency of our method, we extend the micro-architecture by replacing Squeeze-Excite (SE) module with Split-Attention (SA) module [39] in the MBConv block (Fig 2), and denote it as FP-NAS micro-architecture (Table 2, 2nd row). SA module generalizes SE module from one split to multiple splits. However, in the original hand-crafted ResNet models [39], a fixed number of splits (e.g. 2 or 4) is chosen, and SA modules are used within all ResNetXt blocks. We hypothesize it is unnecessary to use SA module everywhere, which will incur computational overhead. Therefore, we make SA module fully searchable by extending the search variable \textit{no. of splits} to have extra choices \{2, 4\}, which means each block group can independently choose whether SA module is used and how many splits to use. Note we do not share the model weights of MBConv block between choices of \textit{no. of splits}, which means the total model weights of the supernet will double as extra choices \{2, 4\} are introduced, and makes the search more challenging. We name the space, which combines FPNetV2-F macro-architecture and FP-NAS micro-architecture, as \textit{FBNetV2-F++} space, which is \(10^3\) larger than FBNetV2-F space.

**FP-NAS spaces.** The largest model in FBNetV2-F++ space only use 122M FLOPS when input size is 128. To demonstrate the efficiency of our search method, we expand the FBNetV2-F macro-architecture in the following aspects. We increase the searchable channels in the block to make it wider. We also increase the repeating times of the block in the group to make it deeper. Last, we increase the input image size to classify the images at higher resolution for better recognition performance. More details of the FP-NAS macro-architectures can be seen in the supplement. By combining the expanded macro-architectures and FP-NAS micro-architecture, we obtain three giant FP-NAS spaces L0-L1 (Table 3), which contain models of different size for us to search. We also use FP-NAS-L to denote the searched models from these spaces.
The original PARSEC [4] uses fixed sampling (FS), and constantly draws $K$ architectures (e.g. 8 or 16). Below we conduct a study in the FPNNetV2-F space to show the choice of $K$ has a significant impact on the search. For FS, in Fig 3a, there is a strong correlation between $K$ and the final architecture quality in terms of Accuracy-To-Complexity (ATC) trade-off on ImageNet-1K validation set. In Fig 3b, a larger $K$ samples more architectures, and the distribution entropy is reduced more substantially, which means learning of the architecture distribution is more effective. In Fig 3c, we show the ImageNet-100 validation accuracy of the most probable architecture at the end of each search epoch. The joint optimization of architecture parameters and model weights is more effective with a larger $K$. More samples help to better estimate the gradients, and leads a faster learning of the distribution, which in turn samples promising architectures more often, and focuses more on updating model weights associated with them. In Fig 3d, the total sampled architectures and the search time by FS with $K = 14$ is $3.5 \times$ and $2.1 \times$ more compared with those by FS with $K = 4$, indicting the computational cost of the search with FS increases almost linearly in $K$.

We also experiment adaptive sampling (AS) with different $\lambda \in \{ \frac{1}{16}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2} \}$. AS adjusts the sample size on the fly. For example, AS with $\lambda = \frac{1}{2}$ draws 14 samples in the beginning, on par with FS with $K = 14$. However, as distribution entropy decreases, it will reduce the samples to save computation, and only draw a single sample at the end of search. In Fig 3a, AS with $\lambda = \frac{1}{2}$ can search an architecture with ATC trade-off similar to that of the one from FS with $K = 14$ using much fewer GPU-days. A larger choice of $\lambda = \frac{1}{4}$ for AS further improves the ATC trade-off. A further larger choice of $\lambda = \frac{1}{2}$ for AS does not improve the ATC trade-off, but will increases the search time. Therefore, we use $\lambda = \frac{1}{2}$ in the following experiments.

In Fig 3b, AS with larger $\lambda$ samples more architectures, and reduces distribution entropy faster. Both $\lambda = \frac{1}{4}$ and $\frac{1}{2}$ can reduce the entropy to a low level at the end. In Fig 3c, AS with both $\lambda = \frac{1}{4}$ and $\frac{1}{2}$ can achieve the high final validation accuracy on ImageNet-100 comparable to that of FS with
where the entropy is lower but not yet converged, the search

The results are shown in Table 4. In small FBNetV2-F space, the entropy at epoch 80 is quite different (30.6 Vs. 54.4). But in the later stage of the search, where the entropy is lower but not yet converged, the search

| Search Space Name | # Architectures | Sampling Method | Model FLOPS (M) | Top-1 Acc (%) |
|-------------------|-----------------|-----------------|-----------------|--------------|
| FBNetV2-F         | $6 \times 10^{25}$ | FS, $K = 14$ | 56               | 68.3         |
|                   |                 | AS, $\lambda = 0.25$ | 58               | 68.6         |
| FBNetV2-F-Fine    | $1 \times 10^{16}$ | FS, $K = 14$ | 50               | 66.3         |
|                   |                 | AS, $\lambda = 0.25$ | 51               | 67.2         |

Table 4: Comparison of models searched in small and large space using two different sampling methods.

Figure 4: Comparing joint-, factorized- and our proposed mixed distributions. (a): The architecture distribution entropy during the search. The beginning part of the search, where the entropy of the factorized distribution is reduced much faster than that of the joint distribution, is highlighted by the dashed box. (b): Total architecture samples and overall search time, which are highly correlated, for different choices of architecture distribution scheduling.

$K = 14$. In Fig 3d, AS with $\lambda = \frac{1}{3}$ samples 60% fewer architectures, and searches 1.8× faster compared with FS with $K = 14$.

5.2.2 FP-NAS Adapts to Search Space Size

In larger search spaces, there are much more architecture choices which requires to draw more samples to explore the space and learn the distribution. For FS, using a constant sample size $K$ will only discover sub-optimal models in larger search space. In contrast, AS with a constant value of $\lambda$ will adjust the sample size based on the distribution entropy, and does not require manual hyper-parameter tuning. To see this, for FS with $K = 14$ and AS with $\lambda = 0.25$, we compare the searched models from FBNetV2-F and FBNetV2-F-Fine space, where the latter is $10^8 \times$ larger. The results are shown in Table 4. In small FBNetV2-F space, the models discovered by two sampling methods have comparable ATC trade-off. However, in larger FBNetV2-F-Fine space, without changing the hyper-parameter of each sampling method, the search with AS discovers a significantly better model with 0.9% higher accuracy.

5.3. Fast Coarse-to-Fine Search

In Fig 4, we first compare the search with joint distribution (JD) only and factorized distribution (FD) only. The search with FD can reduce the entropy much faster than the search with the JD. The entropy at epoch 80 is quite different (30.6 Vs. 54.4). But in the later stage of the search, where the entropy is lower but not yet converged, the search

with FD reduces the entropy slower than that with the JD, which means it struggles to distinguish architectures among a smaller set of candidates at a finer granularity.

In our proposed coarse-to-fine search, we use a schedule of mixed distributions (MD), by starting the search with FD, and later convert it to the JD at search epoch $\theta$. In Fig 4a, we also show results of the search with MD using two different $\theta \in \{80, 150\}$, and also compare with the baseline search using either JD only or FD only. The search with MD can reduce the entropy almost as fast as that with FD at the beginning of the search. After FD is converted into JD for more fine-grained search, it can further reduce the entropy nearly as low as that in the search with JD only. Since the number of sampled architectures is proportional to the entropy of the distribution in our adaptive sampling, the search, which has faster reduction in the distribution entropy, samples fewer architectures, executes fewer forward/backward passes for sampled architectures, and eventually runs faster.

In Fig 4b and Table 5, we show the coarse-to-fine search reduces architecture samples by 9%, runs 1.2× faster than the search using JD only, and does not hurt ATC trade-off. Compared with the original PARSEC, the FP-NAS search with both adaptive sampling and the schedule of mixed distribution reduces samples by 64% and runs 2.1× faster.

5.4. Comparisons with FBNetV2

We search 4 small models in FBNetV2-F space using target FLOPS 60M, 90M, 130MF, and 250MF, respectively, and name them as FP-NAS-S models. We compare with 4 FBNetV2 models (i.e. from S1 to S4), which are searched in the same space. Results are shown in Table 6. Our method not only searches 1.9× to 3.6× faster, but also discovers models with better ATC trade-off. This demonstrates the superior search effectiveness and efficiency of our method. Furthermore, we stress that FBNetV2 method can not be used to search large models due to its excessively large memory footprint which is required to cache all choices of layer operation. In contrast, our FP-NAS method uses much smaller memory footprint and can be used to directly search large models, as we will show later in Section 5.6.

Table 5: Comparing the schedule of architecture distribution and the accuracy of the searched models. Adaptive sampling with $\lambda = \frac{1}{3}$ is always used when different distribution schedules are compared. We report the top-1 accuracy on ImageNet-1K validation set. The search space FBNetV2-F is used. All models in the table use a comparable amount of FLOPS between 58-60M FLOPS.
Table 6: Comparisons with FBNetV2 [33]. Given the same input size, the FBNetV2 models and FP-NAS models here use a similar amount of compute with difference less than 4M FLOPS.

Table 7: Comparison of models searched in FBNetV2-F and FBNetV2-F++ space.

5.5. Searchable Split-Attention Module

We search in FBNetV2-F++ space, where includes searchable Split-Attention (SA) module in MBConv block, and denote the searched models as **FP-NAS-S++** models. In Table 7, we compare them to FP-NAS-S models, which are searched in FBNetV2-F space. We also prepare two variants of FP-NAS-S models, by uniformly replacing the searched SE module with SA module using 2 or 4 splits. The searched FP-NAS-S++ models use a varying number of splits in different MBConv blocks (see model details in the supplement), and achieve significantly better ATC trade-off than FP-NAS-S models and their variants. This highlights the importance of searching the places of inserting SA modules and the number of splits for individual SA modules.

5.6. Searching For Large Models

To demonstrate the scalability of our method, we also search large models in FP-NAS spaces. Specifically, we search 3 models in FP-NAS spaces with different target GFLOPS {0.4, 0.7, 1.0}, and the searched models are denoted as **FP-NAS-L** models. The results are shown in Table 8 and Fig 1, where we compare them with EfficientNet models of similar FLOPS. While both EfficientNet-B0 and FP-NAS-L0 models are searched from scratch, our search runs at least 132× faster and FP-NAS-L0 achieve 0.6% higher top-1 accuracy on ImageNet. Different from EfficientNet-B1/B2, which are obtained by scaling up the EfficientNet-B0 models, our FP-NAS-L1/L2 models are searched from scratch, and improve the accuracy by 0.7% and 0.3%, while reducing the search time by over an order of magnitude.

5.7. Comparisons with Other Methods

FP-NAS can natively search both small and large models. We use simple distillation [11], where the large EfficientNet-B4 model is used as the teacher model, to further improve our L1 and L2 models. In Table 8 and Figure 1, we compare FP-NAS models with others. Our models has shown significantly better ATC trade-off than others. We also compare to BigNAS [38] models with and without using inplace distillation [37] in Table 8. For small model, FP-NAS-S4++ without distillation already works as well as the BigNAS-S model with advanced inplace distillation. For large model, FP-NAS-L2 with vanilla distillation can outperform BigNAS-XL with inplace distillation by 0.7% using less FLOPS.

6. Conclusions

We presented a fast version of the probabilistic NAS. We demonstrate its superior performance by directly searching architectures, including both small and large ones, in large spaces, and validate their high performance on ImageNet.
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Appendices

A. Index

The supplementary materials are organized as follows.
- We present the details of the searched FP-NAS models and visualize them in Section B.
- Details of our training recipe, and comparisons with those used by other methods are presented in Section C.
- Details of FP-NAS search spaces are presented in Section D.
- A study on the supernet warmup is presented in Section E.
- The details of FP-NAS search algorithm is presented in Section F.
- The derivation of gradients for updating architecture parameters is shown in Section G.

B. Understanding FP-NAS Architectures

We use the proposed FP-NAS method to search for a family of models in different sizes. The complete results are shown in Table B.9.

We also visualize two representative FP-NAS models, including FP-NAS-S1++ and FP-NAS-L2 model, in Fig B.5. Compared with hand-crafted models, the searched architectures select more non-uniform choices along kernel size, non-linearity, feature channel and number of splits over MB-Conv blocks.

For example, small kernel size 3 is more favored in the early blocks while large kernel size 5 is more often chosen in the later blocks. This is likely because large kernel size is more computationally expensive and we can only afford to use it in the later blocks where the spatial size of feature map is small (e.g., 14\(^2\), 7\(^2\)). Also in the later blocks, convolution with large kernel size can more effectively capture the global context.

We also find large choices of the number of splits in SA block, such as 2 and 4, are more often used in the later blocks. This is likely because high-level semantic features only emerge in the later blocks, and attention with multiple splits is more needed to attend to certain semantic features relevant to the image content, compared with low-level features in the early blocks where attention is less useful.

C. Training Recipes

When training FP-NAS models, we adopt label smoothing [30] (LS), Auto-Augment [6] (AA), and Exponential Model Averaging (EMA). We study the impact of the training recipe on the testing accuracy by training FP-NAS models under different training recipes. The results are shown in Table C.10.

For AA which augments the training data, it can improve the accuracy of our small models, including S1++ and S4++ models, by 0.2%. It also improves the accuracy of large models, such as L0 and L2 models, by 0.3% and 0.4%, respectively.

Table B.9: The family of FP-NAS models. All results are obtained using one model and a single crop on ImageNet-1K. Column Distill denotes whether model distillation [11] is used to train the model.

| Architecture | Input size | FLOPS(M) | Params(M) | Distill | Top-1 acc (%) |
|--------------|------------|----------|-----------|---------|---------------|
| S1++         | 128\(^2\)  | 66       | 5.9 \(\times\) | ✓       | 70.0          |
| S2++         | 160\(^2\)  | 98       | 5.8 \(\times\) | ×       | 72.2          |
| S3++         | 192\(^2\)  | 147      | 5.8 \(\times\) | ✓       | 74.2          |
| S4++         | 224\(^2\)  | 268      | 6.4 \(\times\) | ×       | 76.6          |
| L0           | 224\(^2\)  | 399      | 11.3 \(\times\) | ✓       | 77.9          |
| L1           | 240\(^2\)  | 728      | 15.8 \(\times\) | ✓       | 80.9          |
| L2           | 256\(^2\)  | 997      | 20.7 \(\times\) | ✓       | 81.6          |

Table C.10: ImageNet top-1 accuracy (%) of FP-NAS models trained with different training recipes. We start with using LS only, and sequentially add AA and EMA.

| Model         | LS | AA | EMA | Top-1 acc (%) |
|---------------|----|----|-----|---------------|
| FP-NAS-S1++   | ✓  | ×  | ✓   | 69.8          |
| FP-NAS-S4++   | ✓  | ×  | ✓   | 76.4          |
| FP-NAS-L0     | ✓  | ✓  | ✓   | 77.6          |
| FP-NAS-L2     | ✓  | ✓  | ✓   | 80.2          |

Table C.11: Comparing training recipe used by different methods. We use the following short-hand notations. LS: label smoothing [30], AA: auto-augmentation [6], EMA: exponential model averaging [32], and SD: stochastic depth [15].
which was shown to be effective in mitigating the difficulties of training deep models, and improve the testing accuracy by 0.3% and 1.4%, respectively.

We also compare our training recipe with that from other methods, and the results are shown in Table C.11. For small models under consideration, including MnasNet [31] and FBNetV2 [33], they are different in whether AA and EMA are used. Although FP-NAS-S++ models are trained with both AA and EMA, the improvement by using either one is much less significant compared with the improvement of FP-NAS-S++ models over other models (See Table 8 in the paper).

For training large FP-NAS-L models, we use LS, AA, and EMA. However, EfficientNet training additionally use Stochastic Depth (SD) [15] with survival probability 0.8, which was shown to be effective in mitigating the difficulties of training deep models, and improve the testing accuracy [15]. Nevertheless, FP-NAS-L models trained without SD still outperform EfficientNet models by a margin from 0.3% to 0.6% while the architecture search is substantially faster.

**D. FP-NAS Search Spaces**

In the Table D.12, we introduce three FP-NAS search spaces from L0 to L2. They share the same FP-NAS micro-architecture, but have different macro-architectures, which are shown in Table D.13, D.14, and D.15, respectively.

**E. SuperNet Warmup**

In our experiments, we fix the architecture hyperparameters while only updating the model weights at the beginning of search for a number of epochs. This is to warm-up the supernet by uniformly sampling architectures from the initial distribution, and update model weights associated with them. Compared with randomly initialized model weights, the updated weights lead to a better estimation of the data likelihood $P(y|X, \omega, A_k)$ of the sampled architectures $\{A_k\}$ and therefore a better estimation of the gradients for updating architecture parameters.

In a study where architecture is searched in FBNetV2-F
The macro-architecture of FP-NAS-L1 search space. It is used to search for FP-NAS-L1 architecture.

| Max Input ($S^2 \times C$) | Operator | Expansion | Channel | Repeat | Stride |
|---------------------------|----------|-----------|----------|--------|--------|
| $256^2 \times 3$          | conv $3 \times 3$ | -          | 24       | 1      | 2      |
| $128^2 \times 24$         | MBConv   | (1, 5, 6.0, 0.75) | (16, 40, 8) | 1 1   |
| $128^2 \times 40$         | MBConv   | (1, 5, 6.0, 0.75) | (24, 40, 8) | 2 2   |
| $64^2 \times 40$          | MBConv   | (1, 5, 6.0, 0.75) | (24, 40, 8) | 2 2   |
| $64^2 \times 40$          | MBConv   | (1, 5, 6.0, 0.75) | (24, 72, 8) | 3 2   |
| $32^2 \times 72$          | MBConv   | (1, 5, 6.0, 0.75) | (24, 72, 8) | 2 1   |
| $32^2 \times 72$          | MBConv   | (1, 5, 6.0, 0.75) | (64, 120, 16) | 3 2   |
| $16^2 \times 120$         | MBConv   | (1, 5, 6.0, 0.75) | (88, 168, 16) | 3 1   |
| $16^2 \times 120$         | MBConv   | (1, 5, 6.0, 0.75) | (136, 272, 16) | 2 2   |
| $8^2 \times 272$          | MBConv   | (1, 5, 6.0, 0.75) | (136, 272, 16) | 2 1   |
| $8^2 \times 272$          | MBConv   | (1, 5, 6.0, 0.75) | (208, 336, 16) | 2 1   |
| $8^2 \times 336$          | MBConv   | (1, 5, 6.0, 0.75) | (208, 336, 16) | 2 1   |

Table D.15: The macro-architecture of FP-NAS-L2 search space. It is used to search for FP-NAS-L2 architecture.

| Max Input ($S^2 \times C$) | Operator | Expansion | Channel | Repeat | Stride |
|---------------------------|----------|-----------|----------|--------|--------|
| $256^2 \times 3$          | conv $3 \times 3$ | -          | 24       | 1      | 2      |
| $128^2 \times 24$         | MBConv   | (1, 5, 6.0, 0.75) | (16, 40, 8) | 1 1   |
| $128^2 \times 40$         | MBConv   | (1, 5, 6.0, 0.75) | (24, 40, 8) | 2 2   |
| $64^2 \times 40$          | MBConv   | (1, 5, 6.0, 0.75) | (24, 40, 8) | 2 2   |
| $64^2 \times 40$          | MBConv   | (1, 5, 6.0, 0.75) | (24, 72, 8) | 3 2   |
| $32^2 \times 72$          | MBConv   | (1, 5, 6.0, 0.75) | (24, 72, 8) | 2 1   |
| $32^2 \times 72$          | MBConv   | (1, 5, 6.0, 0.75) | (64, 120, 16) | 3 2   |
| $16^2 \times 120$         | MBConv   | (1, 5, 6.0, 0.75) | (88, 168, 16) | 3 1   |
| $16^2 \times 120$         | MBConv   | (1, 5, 6.0, 0.75) | (136, 272, 16) | 2 2   |
| $8^2 \times 272$          | MBConv   | (1, 5, 6.0, 0.75) | (136, 272, 16) | 2 1   |
| $8^2 \times 272$          | MBConv   | (1, 5, 6.0, 0.75) | (208, 336, 16) | 2 1   |
| $8^2 \times 336$          | MBConv   | (1, 5, 6.0, 0.75) | (208, 336, 16) | 2 1   |

Table E.16: Comparing searched architectures when supernet warmup is used or not.

| SuperNet Warmup | FLOPS (M) | Top-1 Accuracy (%) |
|-----------------|-----------|--------------------|
| $\times$        | 59        | 67.8               |
| $\sqrt{\times}$ | 58        | 68.6               |

In each search epoch, we iteratively take training- and validation batch data, adaptively sample a number of $K$ architectures based on the distribution entropy. For each sampled architecture, we compute the gradients, accumulate them over all sampled architectures, and finally use the gradients to update both model weights $\omega$ and architecture hyper-parameters $\alpha$. At the end of the search, we return the most probable architecture $A^*$, which will be trained from scratch for final evaluation.

G. Derivation of Gradients for Updating Architecture Parameters

In Eqn (7) of the paper, we presented how to compute the gradient w.r.t architecture hyper-parameters $\alpha$. The full derivation is shown below. First, the cost-aware loss function is defined as follows.

$$
\mathcal{L}(\omega, \alpha) = -\log P(y|X, \omega, \alpha) + \beta \log C(\alpha) \quad (8)
$$

Then, the gradient w.r.t architecture parameters can be derived as follows.

$$
\nabla_\alpha \mathcal{L}(\omega, \alpha) = \frac{1}{P(y|X, \omega, \alpha)} \int P(y|X, \omega, A) \nabla_\alpha - P(A|\alpha) \, dA + \beta \frac{1}{C(\alpha)} \int C(A) \nabla_\alpha P(A|\alpha) \, dA
$$

$$
\approx \int P(A|\alpha) \left( \frac{P(y|X, \omega, A)}{P(y|X, \omega, \alpha)} - \beta \frac{C(A)}{C(\alpha)} \right) \nabla_\alpha - \log P(A|\alpha) \, dA
$$

$$
\approx \sum_k \left( \frac{P(y|X, \omega, A_k)}{P(y|X, \omega, \alpha)} - \beta \frac{C(A_k)}{C(\alpha)} \right) \nabla_\alpha - \log P(A_k|\alpha)
$$

$$
\approx \sum_k m_k^\alpha \nabla_\alpha - \log P(A_k|\alpha)
$$

$$
\text{where } m_k^\alpha = \frac{P(y|X, \omega, A_k)}{\sum_{k'} P(y|X, \omega, A_{k'})} - \beta \frac{C(A_k)}{\sum_{k'} C(A_{k'})}.
$$

The full pseudo-algorithm of FP-NAS is shown in Algorithm 1. We search for a total of $T$ epochs including the beginning $T_{\omega}$ warmup epochs where only model weights $\omega$ are updated and architecture hyper-parameters $\alpha$ are fixed. In each search epoch, we iteratively take training- and validation
Algorithm 1: Pseudocode of Fast Probabilistic Neural Architecture Search.

Result: The most probable architecture $A^*$

Input:
- $\{(X_{\text{train}}^i, y_{\text{train}}^i)\}_{i=1}^N$: training batch data
- $\{(X_{\text{val}}^i, y_{\text{val}}^i)\}_{i=1}^N$: validation batch data
- $\omega$: model weights
- $\alpha$: architecture parameters
- $P(A|\alpha)$: architecture distribution
- $T$: total search epochs
- $T_w$: warm-up epochs
- $T_\theta$: epoch number where $P(A|\alpha)$ is converted from factorized- into joint distribution
- $\lambda$: scaling factor in adaptive sampling

Initialization:
- $\omega \leftarrow$ random initialization
- $\alpha \leftarrow 0$

// iterate over epochs
for $t = 1, \ldots, T$ do
  // iterate over batch data
  for $i = 1, \ldots, N$ do
    compute entropy $H$ of distribution $P(A|\alpha)$
    update sample size $K = \lambda H(P(A|\alpha))$
    // sample architectures
    for $k = 1, \ldots, K$ do
      sample architecture $A_k$ from distribution $P(A|\alpha)$
      compute data-likelihood $P(y_{\text{val}}^i|X_{\text{val}}^i, \omega, A_k)$ and architecture cost $C(A_k)$
    end
    reset gradients $g_\omega \leftarrow 0$, $g_\alpha \leftarrow 0$
    // iterate over sampled architectures, and accumulate gradients
    for $k = 1, \ldots, K$ do
      compute architecture weights $m^\omega_k = P(y_{\text{val}}^i|X_{\text{val}}^i, \omega, A_k) / \sum_k P(y_{\text{val}}^i|X_{\text{val}}^i, \omega, A_k)$
      compute architecture weights $m^\alpha_k = m^\omega_k - \beta C(A_k) / \sum_k C(A_k)$
      $g_\omega \leftarrow g_\omega + m^\omega_k \nabla_\omega - \log P(y_{\text{train}}^i|X_{\text{train}}^i, \omega, A_k)$
      if $t > T_w$ then
        $g_\omega \leftarrow g_\omega + m^\omega_k \nabla_\omega - \log P(A_k|\alpha)$
      end
    end
    update $\omega$ by gradient $g_\omega$
    update $\alpha$ by gradient $g_\alpha$
  end
  if $t == T_\theta$ then
    convert $P(A|\alpha)$ from factorized- to joint distribution
  end
return the most probable architecture $A^* = \arg\max P(A|\alpha)$