Resource-Constrained Neural Architecture Search on Tabular Datasets

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Abstract

The best neural architecture for a given machine learning problem depends on many factors: not only the complexity and structure of the dataset, but also on resource constraints including latency, compute, energy consumption, etc. Neural architecture search (NAS) for tabular datasets is an important but under-explored problem. Previous NAS algorithms designed for image search spaces incorporate resource constraints directly into the reinforcement learning rewards. In this paper, we argue that search spaces for tabular NAS pose considerable challenges for these existing reward-shaping methods, and propose a new reinforcement learning (RL) controller to address these challenges. Motivated by rejection sampling, when we sample candidate architectures during a search, we immediately discard any architecture that violates our resource constraints. We use a Monte-Carlo-based correction to our RL policy gradient update to account for this extra filtering step. Results on several tabular datasets show TabNAS, the proposed approach, efficiently finds high-quality models that satisfy the given resource constraints.

1 Introduction

It is often observed that to make a machine learning model better, one can scale it up. However this is not always possible when machine learning models are deployed since larger networks are also more expensive as measured by inference time, memory, energy, etc. These costs limit the application of large models: training these models is unsustainable, and inference is often too slow to satisfy end user requirements.

One of the most widespread applications of machine learning in industry is tabular data in, e.g., finance, advertising and medicine. It was only recently that in these applications deep learning was able to outperform classical tree-based models [10, 14].

For vision, optimizing the models to make them suitable for practical deployment often relies on Neural Architecture Search (NAS). Most NAS literature targets these convolutional networks on vision benchmarks [20, 6, 11, 30]. Despite the practical importance of tabular data, NAS research on this topic is quite limited [9, 8].

Weight-sharing allows us to reduce the cost of NAS by training a SuperNet that is the superset of all architecture candidates [4]. This trained SuperNet is then used to estimate the quality of the individual architectures, the so-called child networks, by only activating a subset of components of that architecture and running an evaluation. To efficiently find the most promising child networks, Reinforcement Learning (RL) has shown to be effective [23, 6, 5] on vision problems.

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In our experiments, we observe that a direct application of the vision approaches for tabular data is suboptimal. We started from the TuNAS [5] approach from vision and observed that this struggled to find the optimal architectures for tabular datasets. The failure is caused by the interaction of the search space and the RL controller. In vision, a popular approach is to use a factorized RL controller, which assumes that all choices can be made independently. The search space consists of a limited number of options per layer. In tabular data, we need more options per layer, but there are fewer layers overall. Feedforward networks with bottleneck structures often outperform other feed-forward networks of similar size on tabular data. In such a bottleneck architecture, there exists at least one hidden layer that is much narrower than its preceding and following layers. A popular hypothesis is that its weights resemble the low-rank factors of a wider network, and thus mimics the behavior of the latter with less cost [17, 7]. These bottleneck structures often have a a very good tradeoff between cost and quality (more examples in Appendix [B.2.1 Table[3]], but finding these bottleneck structures is difficult for a factorized RL controller. To understand why, we consider the following toy example with 2 layers, illustrated in Figure[1]. For the each layer, we can choose a layer size of 2, 3 or 4 and the maximum compute budget is set to 25. The optimal solution is to set the size of layer 1 to 4 and layer 2 to 2. Finding this solution is difficult with a cost penalty. The RL controller is initialized with uniform probabilities. As a result, it is quite likely that the RL controller will initially be penalized heavily when choosing option 4 for the first layer, since two thirds of the choices for the second layer will result in a model that is too expensive. As a result, option 4 for the first layer is quickly discarded by the RL controller and we get stuck in a local optimum.

To circumvent this problem, one could attempt to learn a non-factorized probability distribution. However, this requires a more complicated model, e.g., an LSTM, that is often more difficult to tune. We propose a different solution inspired by rejection sampling. We only update the RL controller when the sampled model satisfies our cost constraint. The RL controller is then discouraged from sampling poor models within the cost constraint and encouraged to sample the high quality models. Rather than penalizing models which violates the cost constraints, the controller silently discards them, thereby circumventing the local optimum.

Our contributions can be summarized as follows:

- We first identify failure cases of existing resource-aware NAS methods on tabular data, and link these cases to the cost penalty in the reward.
- We then propose and evaluate an alternative: a rejection mechanism which ensures that the RL controller can only select architectures that satisfy the user-specified resource constraint. Instead of reward shaping, this extra rejection step allows the RL controller to explore parts of the search space which would otherwise be overlooked.
- The rejection mechanism also introduces a systematic bias into the RL gradient updates, which can skew the search results. To compensate for this bias, we introduce a theoretically motivated and empirically effective correction into our gradient updates. This correction can be computed exactly for small search spaces, and we show how to efficiently approximate it with Monte-Carlo sampling when the space is large.

These contributions form TabNAS, our RL-based weight-sharing NAS with the rejection-based reward that can robustly and efficiently find a feasible architecture that has optimal performance within the resource constraint. Figure[2] shows an example.

2 Notation and Terminology

Math basics. We define $[n] = \{1, \ldots, n\}$ for a positive integer $n$. With a Boolean variable $X$, the indicator function $1(X)$ equals 1 if $X$ is true, and 0 otherwise. $|S|$ denotes the cardinality of a set $S$; stop_grad($f$) denotes the constant value (with gradient 0) corresponding to a differentiable quantity $f$, and is equivalent to tensorflow.stop_gradient($f$) in TensorFlow [1] or $f$.detach() in PyTorch [22]. $\subseteq$ and $\subset$ denote subset and strict subset, respectively. $\nabla$ denotes the gradient with respect to the variable in the context.

Weight, architecture, and hyperparameter. We use weights to refer to the parameters of the
Figure 1: A toy example for tabular NAS in the 2-layer search space with a 2-dimensional input and a limit of 25 parameters. The left half shows the number of parameters and loss of each candidate architecture in the search space. The infeasible architectures have striped patch in the corresponding cells. The bottom left cell squared in bold is the global optimal architecture with hidden size 1 = 4 and hidden size 2 = 2. The right half shows the change of sampling probabilities in weight-sharing NAS with different RL rewards. Each cell represents an architecture; the sampling probability value is shown both as a percentage in the cell, and with the color intensity indicated by the right colorbar. The orange bars on the top and right sides show the sampling probability distribution among size candidates for each layer. With the Abs Reward, the sampling probability of each architecture is the product of sampling probabilities of its layer sizes; with the rejection-based reward, the sampling probability of an infeasible architecture is 0, and that of a feasible architecture gets reweighted by the sum of probabilities of all feasible architectures. At epoch 500, the cell squared in bold shows the architecture picked by the corresponding RL controller. RL with the Abs Reward $Q(x) + \beta|T(x)/T_0 - 1|$ proposed in TuNAS [5] either converges to a feasible but suboptimal architecture ($\beta = -2$, middle row) or violates the resource constraint ($\beta = -1$, top row). Other latency-aware reward functions show similar failures. In contrast, our new rejection-based controller converges to the optimal solution (bottom row).
Figure 2: Rejection-based reward distributionally outperforms random search and resource-aware AbS Reward on the Criteo dataset within a 3-layer search space. All error bars and shaded regions are 95% confidence intervals. The x axis is the time relevant to training a single architecture in the search space. Results of random sampling comes from 100 independent runs on 50 architectures within the number of parameters range. The result of each RL method comes from 5 independent runs. The skyline is the performance of 3 independent retrains of the best architecture that is found by 3 independent exhaustive searches. More details in Appendix B.2.3.

neural network and are trained in the neural network training. The architecture of a neural network is the structure of how nodes are connected; examples of architectural choices are hidden layer sizes and activation types. Hyperparameters are the the non-architectural parameters that control the training process of either stand-alone training or RL, including learning rate, optimizer type, optimizer parameters, etc.

Neural architecture. A neural network with specified architecture and hyperparameters is called a model. We only consider fully-connected feedforward networks (FFNs) in this paper, since they can already achieve SOTA performance on tabular datasets [14]. The number of hidden nodes after each weight matrix and activation function is called a hidden layer size. We denote a single network in our search space with hyphen-connected choices. For example, when searching for hidden layer sizes, in the space of 3-hidden-layer ReLU networks, 32-144-24 denotes the candidate where the sizes of the first, second and third hidden layers are 32, 144 and 24, respectively. We only search for ReLU networks; for brevity, we will not mention the activation function type in the sequel.

Loss-resource tradeoff and reference architectures. As shown in the tradeoff plots in Figure 3 within the hidden layer size search space, the validation loss in general decreases with the increase of the number of parameters, giving the loss-resource tradeoff. Loss and number of parameters can be understood as two costs for the NAS problem. Thus there are Pareto-optimal models that achieve the smallest loss among all models with a given bound on the number of parameters. With an architecture that outperforms others with a similar or fewer number of parameters, we do resource-constrained NAS with the number of parameters of this architecture as the resource target or constraint. We call this architecture the reference architecture (or reference) of NAS, and its performance the reference performance. We do NAS with the goal of matching (the size and performance of) the reference. Note that the RL controller only has knowledge of the number of parameters of the reference, and is not informed of its hidden layer sizes.

Search space. When searching $L$-layer networks, we use capital letters like $X = X_1 \cdots X_L$ to denote the random variable of sampled architectures, in which $X_i$ is the random variable for the size of the $i$-th layer. We use lowercase letters like $x = x_1 \cdots x_L$ to denote an architecture sampled from the distribution over $X$, in which $x_i$ is an instance of the $i$-th layer size. When there are multiple samples drawn, we use a bracketed superscript to denote the index over samples: $x^{(k)}$ denotes the $k$-th sample. The search space $S = \{s_{ij}\}_{i \in [L], j \in [C_i]}$ has $C_i$ choices for the $i$-th hidden layer, in which $s_{ij}$ is the $j$-th choice for the size of the $i$-th hidden layer: for example, when searching for a one-hidden-layer network with size candidates $\{5, 10, 15\}$, we have $s_{13} = 15$. 

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Figure 3: Tradeoff between loss and number of parameters on Criteo within a 3-layer search space. The search space and Pareto-optimal architectures are shown in Appendix B.2.1. We use logistic loss as the loss metric. When training each architecture 5 times, the standard deviation (std) across different runs is 0.0002, meaning that the architectures whose performance difference is larger than $2 \times \text{std}$ are qualitatively different with high probability.

**Reinforcement learning.** The RL algorithm learns the set of logits $\{\ell_{ij}\}_{i \in \mathcal{L}, j \in \mathcal{C}_i}$, in which $\ell_{ij}$ is the logit associated with the $j$-th choice for the $i$-th hidden layer. With a fully factorized distribution of layer sizes (we learn a separate distribution for each layer), the probability of sampling the $j$-th choice for the $i$-th layer $p_{ij}$ is given by the SoftMax function: $p_{ij} = \exp(\ell_{ij}) / \sum_{j \in \mathcal{C}_i} \exp(\ell_{ij})$. In each RL step, we sample an architecture $y$ to compute the single-step RL objective $J(y)$, and update the logits with $\nabla J(y)$: an unbiased estimate of the gradient of the RL value function.

**Resource metric and number of parameters.** We use the number of parameters, which can be easily computed for neural networks, as a cost metric in this paper. Our approach does not depend on the specific cost used.

# 3 Methodology

The methodologies we use for NAS can be decomposed into three main components: weight-sharing with layer warmup, REINFORCE with one-shot search, and Monte Carlo (MC) sampling with rejection.

As an overview, our method starts with a SuperNet, which is a network that layer-wise has width to be the largest choice within the search space. We first stochastically update the weights of the entire SuperNet to “warm up” over the first 25% of search epochs. Then we alternate between updating the shared model weights (which are used to estimate the quality of different child models) and the RL controller (which focuses the search on the most promising parts of the space). In each iteration, we first sample a child network from the current layer-wise probability distributions and update the corresponding weights within the SuperNet (weight update), then sample another child network to update the layerwise logits that give the probability distributions (RL update). The latter RL update is only performed if the sampled network is feasible, in which case we use rejection with MC sampling to update the logits with a sampling probability conditional on the feasible set.

To avoid overfitting, we split the labelled portion of a dataset into training and validation splits. Weight updates are carried out on the training split; RL updates are performed on the validation split.

## 3.1 Weight Sharing with Layer Warmup

The weight-sharing approach has shown success on various computer vision tasks and NAS benchmarks [23, 4, 6, 5]. To do search for an FFN on tabular datasets, we build a SuperNet where the size of each hidden layer is the largest value in the search space. Figure 4 shows an example. When we sample a child network with a hidden layer size $\ell_i$ smaller than the SuperNet, we only use the first $\ell_i$ hidden nodes in that layer to compute the output in the forward pass. In weight updates, only the weights in the child network are updated in the backward pass. In RL updates, only the weights of the child network are used to estimate the quality reward that is used to update logits.
In weight-sharing NAS, warmup helps to ensure that the SuperNet weights are sufficiently trained to properly guide the RL updates \[5\]. With probability \( p \), we train all weights of the SuperNet, and with probability \( 1 - p \) we only train the weights of a random child model. When we run architecture searches for FFNs, we do warmup in the first 25% epochs, during which the probability \( p \) linearly decays from 1 to 0 (Figure 5(a)). The RL controller is disabled during this period.

3.2 One-Shot Training and REINFORCE

We do NAS on FFNs with a REINFORCE-based algorithm. Previous works have used this type of algorithm to search for convolutional networks on vision tasks \[26, 6, 5\].

When searching for \( L \)-layer FFNs, we learn a separate probability distribution over \( C_i \) size candidates for each layer. The distribution is given by \( C_i \) logits via the SoftMax function. Each layer has its own independent set of logits. With \( C_i \) choices for the \( i \)th layer, where \( i = 1, 2, \ldots, L \), there are \( \prod_{i \in [L]} C_i \) candidate networks in the search space but only \( \sum_{i \in [L]} C_i \) logits to learn. This technique significantly reduces the difficulty of RL and makes the NAS problem practically tractable \[6, 5\].

The REINFORCE-based algorithm trains the SuperNet weights and learns the logits \( \{\ell_{ij}\}_{i \in [L], j \in [C_i]} \) that give the sampling probabilities \( \{\ell_{ij}\}_{i \in [L], j \in [C_i]} \) over size candidates by alternating between weight and RL updates. In each iteration, we first sample a child network \( x \) from the SuperNet and compute its training loss in the forward pass. Then we update the weights in the child network with gradients of the training loss computed in the backward pass. This weight update step trains the weights of the sampled network. The weights in the architectures with larger sampling probabilities are sampled and thus trained more often. We then update the logits for the RL controller by sampling a child network \( y \) that is independent of the network \( x \) from the same layerwise distributions, compute the quality reward \( Q(y) \) as \( 1 - \text{loss}(y) \) on the validation set, and then update the logits with the gradient of \( J(y) = \text{stop}_\text{grad}(Q(y) - \bar{Q}) \log P(y) \): the product of the advantage of the current network’s reward over past rewards (usually an exponential moving average) and the log-probability of the current sample.

The alternation creates a positive feedback loop that trains the weights and updates the logits of the large-probability child networks; thus the layer-wise sampling probabilities gradually converge to more deterministic distributions, under which one or several architectures are finally selected.

Details of a resource-oblivious version is shown as Algorithm 1 in Appendix A, which does not take into account a resource constraint. In Section 3.3, we show an algorithm that combines Monte-Carlo sampling with rejection sampling, which serves as a subroutine of Algorithm 1 by replacing the probability in \( J(y) \) with a conditional version.
3.3 Rejection-Based Reward with MC Sampling

Only a subset of the architectures in the search space $S$ will satisfy our resource constraints, $V$ denotes this set of feasible architectures. To find a feasible architecture, a resource target $T_0$ is often used in an RL reward. Given an architecture $y$, a latency-aware reward combines its quality $Q(y)$ and resource consumption $T(y)$ into a single reward. MnasNet [26] proposes the reward functions $Q(y) \times (T(y) / T_0)^\beta$ and $Q(y) \times \max\{1, (T(y) / T_0)^\beta\}$ while TuNAS [5] proposes the absolute value reward (or Abs Reward) $Q(y) + \beta |T(y) / T_0 - 1|$. In these approaches $\beta$ is a hyperparameter that needs careful tuning. The idea behind these reward functions is to encourage models with high quality with respect to the resource target.

We found that in tabular data experiments, RL controllers using these resource-aware rewards above can struggle to discover bottleneck structures — where we select a large number of filters for the $i$th layer of the network but a small number of filters for the $i + 1$st layer. Figure 4 in Section 4.1 shows a toy example in the search space where we know the validation losses of each child network and only train the RL controller for 200 steps. The optimal network is 4-2 among architectures with no more than 25, but the RL controller rarely chooses it. In Section 4.1 we show examples of this on real datasets.

Such a phenomenon reveals a gap between the true distribution we want to sample from and the distributions given by factorized search space that we are truly sampling from:

- We only want to sample from the set of feasible architectures $V$, whose distribution is $\{P(y | y \in V)\}_{y \in V}$. The number of parameters (or another resource metric) of an architecture, and thus its feasibility, is determined jointly by the sizes of all layers.
- On the other hand, the factorized search space determines that we learn a separate (independent) probability distribution for the choices of each layer. While this distribution is efficient to learn, the independence assumption makes it difficult for a RL controller with a resource-aware reward to choose a bottleneck structure. A bottleneck requires the controller to select large sizes for some layers and small layer sizes for others. But decisions for different layers are made independently, and both very large and very small layer sizes, when selected independently of each other, have very negative expected rewards. Small layers are likely to have suboptimal quality, and large layers are likely to exceed the resource constraints.

To bridge the gap and efficiently learn layerwise distributions that take into account the architecture feasibility, we propose a rejection-based RL reward for Algorithm 1. We next sketch the idea; detailed pseudocode is provided as Algorithm 2 in Appendix A.

REINFORCE optimizes a set of logits $\{\ell_{ij} \}_{i \in |L|, j \in |C|}$ which define a probability distribution $p$ over architectures. In the original REINFORCE algorithm, we sample a random architecture $y$ from $p$ and then estimate its quality $Q(y)$. Updates to the logits $\ell_{ij}$ take the form $\ell_{ij} \leftarrow \ell_{ij} + \eta \frac{\partial}{\partial \ell_{ij}} J(y)$, where $\eta$ is the learning rate,

$$J(y) = \text{stop}_\text{grad}(Q(y) - \bar{Q}) \cdot \log P(y)$$

and $\bar{Q}$ is a moving average of recent rewards. If $y$ is better (resp. worse) than average then $Q(y) - \bar{Q}$ will be positive (resp. negative), so the REINFORCE update will increase (resp. decrease) the probability of sampling the same architecture in the future.

In our new REINFORCE variant, motivated by rejection sampling, we skip the REINFORCE update to the logits unless $y$ is feasible. And if $y$ is feasible, we replace the probability $P(y)$ in the REINFORCE update equation with the conditional probability $P(y | y \in V) = P(y) / P(y \in V)$. So $J(y)$ becomes

$$J(y) = \text{stop}_\text{grad}(Q(y) - \bar{Q}) \cdot \log [P(y) / P(y \in V)].$$

We can compute the probability of sampling a feasible architecture $P(V) := P(y \in V)$ exactly when the search space is small, but that becomes prohibitively expensive when the space is large. In the latter case, we replace the exact probability $P(y)$ with a differential approximation $\hat{P}(y)$ obtained using Monte-Carlo (MC) sampling. In each RL step, we sample $N$ architectures $\{z^{(k)}\}_{k \in [N]}$ within the search space with a
Figure 5: Example layer warmup and valid probabilities. Figure 5(a) shows our schedule of layer warmup probabilities: linearly decay from 1 to 0 in the first 25% epochs. Figure 5(b) shows an example of the change of true and estimated valid probabilities ($P(V)$ and $\hat{P}(V)$) in a successful search, with 8,000 architectures in the search space and the number of Monte-Carlo samples $N = 1024$. Both probabilities are (nearly) constant during warmup before RL starts, then start to increase when the RL starts because of rejection sampling.

$$\hat{P}(V) = \frac{1}{N} \sum_{k \in [N]} p^{(k)} \cdot q^{(k)} \cdot 1(z^{(k)} \in V)$$

as an estimate of $P(V)$. For each $k \in [N]$, $p^{(k)}$ is the probability of sampling $z^{(k)}$ with the factorized layerwise distributions, and is thus differentiable with respect to the logits. In contrast, $q^{(k)}$ is the probability of sampling $z^{(k)}$ with the proposal distribution, and is therefore non-differentiable.

We show $\hat{P}(V)$ is an unbiased and consistent estimate of $P(V)$, and $\nabla \log[P(y)/\hat{P}(V)]$ is a consistent estimate of $\nabla \log[P(y | y \in V)]$ (Appendix C). A larger $N$ gives better results (Section 3); in our experiments, we need smaller than the size of the sample space to get a faithful estimate (Figure 5(b), Section 4.3 and Appendix C) because neighboring RL steps can correct the estimates of each other. We set $q = \text{stop\_grad}(p)$ in our experiments for convenience: use the current distribution over architectures for MC sampling. Other distributions that have a larger support on $V$ may be used to reduce the sampling variance (Appendix C).

At the end of NAS, we pick the layer sizes with largest sampling probabilities as the found architecture if the layerwise distributions are deterministic, or sample the distributions $m$ times and pick $n$ feasible architectures with the largest number of parameters if not. Appendix A Algorithm 3 provides the full details of this procedure. Although it is cheap to use larger values, we find $m = 500$ and $n \leq 3$ suffice to find an architecture that can match the reference architecture in our experiments.

In practice, we find that the distributions often (almost) converge after $2\times$ of the number of epochs used to train stand-alone child networks, while the distributions are often informative enough after $1\times$ epochs, in the sense that the architectures found by Algorithm 3 are competitive.

Figure 1 show that our rejection-based method finds the best feasible architecture, 4-2, in our toy example, when using the $\hat{P}(V)$ estimated by MC sampling.

4 Experimental Results

We ran all experiments using TensorFlow on a Cloud TPU v2 with 8 cores. We use a 1,027-dimensional input representation for Criteo, 180 features for Volkert and 128 features for Aloi\textsuperscript{1}. More experiment setup details can be found in Appendix B.

\textsuperscript{1}Our paper takes these features as given. It is worth noting that methods proposed in feature engineering works like [16] and [17] are complementary to and can work together with TabNAS.
4.1 When do Previous RL Rewards Fail?

Section 3.3 discussed the resource-aware RL rewards and highlighted a potential failure case. In this section, we show several failure cases of the resource-aware rewards \( Q(x) + \beta |T(x)/T_0 - 1| \) Abs Reward, the target for the reward was 41,153 parameters. Repeated runs of the same search find the same architecture. Figure 6(d) shows the change of validation losses across 5 retraining runs of 32-64-96 (NAS-found) and 32-144-24 (reference).

4.1.1 Criteo – 3 Layer Search Space

We use the 32-144-24 reference architecture, which has 41,153 parameters. Figure 3 gives an overview of the costs and the losses of all architectures in the search space. The search space requires us to choose one of 20 possible sizes for each hidden layer in the network; details are discussed in Appendix C. We set the maximum inference cost to 42,000 parameters. The search has 1.7× the cost of a stand-alone training run.

Failure of latency rewards. Figure 6 shows the sampling probabilities from the search when using the Abs Reward \( Q(x) + \beta |T(x)/T_0 - 1| \), and the retraining performance of the found architecture 32-64-96.

In Figures 6(a)–6(c) we can see that the sampling probabilities for the different choices are uniform during warmup and then converge quickly. The final selected model (32-64-96) is much worse than the reference model (32-144-24) even though the reference model is actually less expensive. We also observed similar failures for the MnasNet rewards. With the MnasNet rewards, the RL controller also struggles to find a model within ±5% of the constraint despite a grid search of the RL parameters (details in Appendix C). In both cases, almost all found models are worse than the reference architecture.

The RL controller is to blame. To verify that a low quality SuperNet was not the culprit, we trained a SuperNet without updating the RL controller, and manually inspected the quality of the resulting SuperNet. The sampling probabilities for the RL controller remained uniform throughout the search; the rest of the training setup was kept the same. At the end of the training, we compare two sets of losses on each of the child networks: the validation loss from the SuperNet (one-shot loss), and the validation loss from training the child network from scratch. Figure 7(a) shows that there is a strong correlation between these accuracies; Figure 7(b) shows RL that starts from the sufficiently trained SuperNet weights in 7(a) still chooses the suboptimal choice 64. This suggests that the suboptimal search results on Criteo are likely due to issues with the RL controller, rather than issues with the one-shot model weights. In a 3 layer search space we can actually find good models without the RL controller, but in a 5 layer search space, we found an RL controller whose training is interleaved with the SuperNet is important to achieve good results.
Figure 7: SuperNet calibration on Criteo among 3-layer networks (with search space in Appendix B), and the Layer 2 change of probabilities in a search with the same number of epochs for only SuperNet training. The y coordinates in Figure (a) are from a SuperNet trained with the same hyperparameters as the search in Figure 6 except that there are no RL updates in the first 60 epochs; the x coordinates are from stand-alone training of architectures with performance standard deviation 0.0003, with each errorbar spanning a range of 0.0006. Figure (a) has a 0.96 Pearson correlation coefficient.

Figure 8: On Volkert, the retrain performance of two $Q(x) + \beta|T(x)/T_0 - 1|$-found architectures versus the 48-160-32-144 reference. Each architecture is trained 5 times with the same setting. The plots of layer-wise sampling probabilities like Figure 6(a)–6(c) are omitted for brevity.

4.1.2 Volkert – 4 Layer Search Space

We search for 4-layer and 9-layer networks on the Volkert dataset\footnote{https://www.openml.org/d/41166}; details are in Appendix C. For resource-aware RL rewards, we ran a grid search over the RL learning rate and $\beta$ hyperparameter. The reference architecture for the 4 layer search space is 48-160-32-144 with 27,882 parameters. Despite a hyperparameter grid search, it was difficult to find models with the right target cost reliably using the MnasNet rewards. Using the Abs Reward (Figure 8), searched models met the target cost but their quality was suboptimal, and the trend is similar to what has been shown in the toy example (Figure 1): a smaller $|\beta|$ gives an infeasible architecture that is beyond the reference number of parameters, and a larger $|\beta|$ gives an architecture that is feasible but suboptimal.

4.1.3 A Common Failure Pattern

Looking back at the failure modes on Criteo and Volkert, we can see that the reference architectures on which the RL controller with soft constraint fails often have a bottleneck structure. For example, with a 1,027-dimensional input representation, the 32-144-24 reference on Criteo has bottleneck 32; with
Figure 9: Success case: on Criteo in a search space of 3-layer FFNs, Monte-Carlo sampling with rejection eventually finds 32-144-24, the reference architecture, with RL learning rate 0.005 and number of MC samples 3,072. Figure 9(d) shows the change of true and estimated valid probabilities.

180 features, the 30-152-18-36 reference on Volkert has bottleneck 30. More examples can be found in Appendix C. As the example in Section 3.3 shows, the wide hidden layers around the bottlenecks get penalized harder in the search, and it is thus more difficult for RL with the Abs Reward to find a model that can match the reference performance. Also, Appendix B.2.1 shows the Pareto-optimal architectures in the tradeoff points in Figure 3 often have bottleneck structures. This means resource-aware RL rewards in previous NAS practice may be more likely to fail than imagined.

Next in Section 4.2, we show the performance of RL with the rejection-based reward in matching these reference architectures.

4.2 NAS with the Rejection-Based Reward

As introduced in Section 3.3, the rejection-based reward does not introduce an additional resource-aware bias in the RL reward, but rather uses conditional probabilities to update the logits in feasible architectures.

To match the 32-144-24 reference on Criteo, we run the search with the MC-sampling-with-rejection approach for 120 epochs, with RL learning rate 0.005 and number of MC samples \( N = 3072 \).

The RL controller converges to two architectures, 32-160-16 (40,769 parameters, with loss 0.4457 ± 0.0002) and 32-144-24 (41,153 parameters, with loss 0.4455 ± 0.0003), after around 50 epochs of NAS, then oscillates between these two solutions (Figure 9). At the end of the 120-epoch search, we sample from the layerwise distribution and pick the largest feasible architecture, causing us to select the reference architecture 32-144-24. It is clear that this approach does not get stuck in a local optimum immediately.

On the same hardware, the search takes \( 3 \times \) the time of a stand-alone training in Figure 6(d) to finish. As a result, as can be seen in Figure 2, the proposed architecture search method is much more efficient than a random baseline.

4.3 Ablation Studies

We do the ablation studies on Criteo with the 32-144-24 reference. The behavior on other datasets with other reference architectures are similar.

Whether to use \( \hat{P}(V) \) instead of \( P(V) \). The Monte-Carlo (MC) sampling estimates \( P(V) \) with \( \hat{P}(V) \) to save resources. Such estimations are especially efficient when the sample space is large. Empirically, the \( \hat{P}(V) \) estimated with enough MC samples (as described in Appendix E) enables the RL controller to find the same architecture as \( P(V) \), because the \( \hat{P}(V) \) estimated with a large enough number of samples is accurate enough (e.g., Figure 5(b) and 9(d)).

\( \hat{P}(V) \) is estimated with a large enough number of samples (as described in Appendix E) enables the RL controller to find the same architecture as \( P(V) \), because the \( \hat{P}(V) \) estimated with a large enough number of samples is accurate enough (e.g., Figure 5(b) and 9(d)).
Whether to skip infeasible architectures in weight updates. In each iteration of one-shot training and REINFORCE (Appendix \[A\] Algorithm 1) with the rejection mechanism (Appendix \[A\] Algorithm 2), we train the weights in the sampled child network \(x\) regardless of whether \(x\) is feasible. Instead, we may update the weights only when \(x\) is feasible, in a similar rejection mechanism as the RL step. We find this mechanism may mislead the search because of insufficiently trained weights: the rejection-based RL controller can still find qualitatively the best architectures on Criteo with the 32-144-24 or 48-240-24-256-8 reference, but fails with the 48-128-16-112 reference. In the latter case, although the RL controller still finds architectures with bottleneck structures (e.g., 32-384-8-144), the first layer sizes of the found architectures are much smaller, leading to suboptimal performance.

Whether to differentiate through \(\hat{P}(V)\). REINFORCE with rejection has the optimization objective:

\[
J(y) = \text{stop}_\text{grad}(Q(y) - \mathcal{Q}) \cdot \log \frac{P(y)}{P(V)}
\]

To update the RL controller’s logits, we compute \(\nabla J(y)\), which requires a differentiable approximation of \(P(V)\). From a theoretical standpoint, omitting the extra term \(P(V)\) – or using a non-differentiable approximation – will result in biased gradient estimates. Empirically, we ran experiments with multiple variants of our algorithm where we omitted the term \(P(V)\), but found that the quality of the searched architectures was significantly worse.

Strategy for choosing the final architecture after search. When RL finishes, instead of biasing towards architectures with more parameters (Appendix \[A\] Algorithm 3), we may also bias towards those that are feasible and have larger sampling probabilities. We find that when the final distributions are less deterministic, the architectures found by the latter strategy perform worse: for example, the top 3 feasible architectures found with the final distribution in Figure 9 are 32-128-16, 32-160-16 and 32-128-8, and they are all inferior to 32-144-24.

References

[1] Martin Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S. Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Ian Goodfellow, Andrew Harp, Geoffrey Irving, Michael Isard, Yangqing Jia, Rafal Jozefowicz, Lukasz Kaiser, Manjunath Kudlur, Josh Levenberg, Dandelion Mané, Rajat Monga, Sherry Moore, Derek Murray, Chris Olah, Mike Schuster, Jonathon Shlens, Benoit Steiner, Ilya Sutskever, Kunal Talwar, Paul Tucker, Vincent Vanhoucke, Vijay Vasudevan, Fernanda Viégas, Oriol Vinyals, Pete Warden, Martin Wattenberg, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. URL https://www.tensorflow.org/. Software available from tensorflow.org.

[2] Noor Awad, Neeratyoy Mallik, and Frank Hutter. Differential evolution for neural architecture search. \textit{arXiv preprint arXiv:2012.06400}, 2020.

[3] Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. Layer normalization. \textit{arXiv preprint arXiv:1607.06450}, 2016.

[4] Gabriel Bender, Pieter-Jan Kindermans, Barret Zoph, Vijay Vasudevan, and Quoc Le. Understanding and simplifying one-shot architecture search. In \textit{International Conference on Machine Learning}, pages 550–559. PMLR, 2018.

[5] Gabriel Bender, Hanxiao Liu, Bo Chen, Grace Chu, Shuyang Cheng, Pieter-Jan Kindermans, and Quoc V Le. Can weight sharing outperform random architecture search? An investigation with TuNAS. In \textit{Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition}, pages 14323–14332, 2020.

[6] Han Cai, Ligeng Zhu, and Song Han. Proxylessnas: Direct neural architecture search on target task and hardware. \textit{arXiv preprint arXiv:1812.00332}, 2018.

[7] Pei-Hung Chen, Hsiang-Fu Yu, Inderjit Dhillon, and Cho-Jui Hsieh. Drone: Data-aware low-rank compression for large nlp models. \textit{Advances in Neural Information Processing Systems}, 34, 2021.
[8] Romain Egele, Prasanna Balaprakash, Isabelle Guyon, Venkatram Vishwanath, Fangfang Xia, Rick Stevens, and Zhengying Liu. Agebo-tabular: joint neural architecture and hyperparameter search with autotuned data-parallel training for tabular data. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, pages 1–14, 2021.

[9] Nick Erickson, Jonas Mueller, Alexander Shirikov, Hang Zhang, Pedro Larroy, Mu Li, and Alexander Smola. Autogluon-tabular: Robust and accurate automl for structured data. arXiv preprint arXiv:2003.06505, 2020.

[10] Yury Gershniy, Ivan Rubachev, Valentin Khrulkov, and Artem Babenko. Revisiting deep learning models for tabular data. arXiv preprint arXiv:2106.11959, 2021.

[11] Andrew Howard, Mark Sandler, Grace Chu, Liang-Chieh Chen, Bo Chen, Mingxing Tan, Weijun Wang, Yukun Zhu, Ruoming Pang, Vijay Vasudevan, et al. Searching for mobilenetv3. In Proceedings of the IEEE/CVF International Conference on Computer Vision, pages 1314–1324, 2019.

[12] Haifeng Jin, Qingquan Song, and Xia Hu. Auto-keras: An efficient neural architecture search system. In Proceedings of the 25th ACM SIGKDD international conference on knowledge discovery & data mining, pages 1946–1956, 2019.

[13] Donald R Jones, Matthias Schonlau, and William J Welch. Efficient global optimization of expensive black-box functions. Journal of Global optimization, 13(4):455–492, 1998.

[14] Arlind Kadra, Marius Lindauer, Frank Hutter, and Josif Grabocka. Well-tuned simple nets excel on tabular datasets. In Thirty-Fifth Conference on Neural Information Processing Systems, 2021.

[15] Kirthevasan Kandasamy, Willie Neiswanger, Jeff Schneider, Barnabas Poczos, and Eric P Xing. Neural architecture search with bayesian optimisation and optimal transport. Advances in neural information processing systems, 31, 2018.

[16] Farhan Khawar, Xu Hang, Ruiming Tang, Bin Liu, Zhenguo Li, and Xiuying He. Autofeature: Searching for feature interactions and their architectures for click-through rate prediction. In Proceedings of the 29th ACM International Conference on Information & Knowledge Management, pages 625–634, 2020.

[17] Mikhail Khodak, Neil A. Tenenholtz, Lester Mackey, and Nicolò Fusi. Initialization and regularization of factorized neural layers. In Proceedings of the 10th International Conference on Learning Representations, 2021.

[18] Bin Liu, Chenxu Zhu, Guilin Li, Weinan Zhang, Jincai Lai, Ruiming Tang, Xiuqiang He, Zhenguo Li, and Yong Yu. Autofis: Automatic feature interaction selection in factorization models for click-through rate prediction. In Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pages 2636–2645, 2020.

[19] Chenxi Liu, Barret Zoph, Maxim Neumann, Jonathon Shlens, Wei Hua, Li-Jia Li, Li Fei-Fei, Alan Yuille, Jonathan Huang, and Kevin Murphy. Progressive neural architecture search. In Proceedings of the European conference on computer vision (ECCV), pages 19–34, 2018.

[20] Hanxiao Liu, Karen Simonyan, and Yiming Yang. Darts: Differentiable architecture search. arXiv preprint arXiv:1806.09055, 2018.

[21] Jonas Močkus. On bayesian methods for seeking the extremum. In Optimization techniques IFIP technical conference, pages 400–404. Springer, 1975.

[22] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. Advances in neural information processing systems, 32:8026–8037, 2019.

[23] Hieu Pham, Melody Guan, Barret Zoph, Quoc Le, and Jeff Dean. Efficient neural architecture search
via parameters sharing. In *International Conference on Machine Learning*, pages 4095–4104. PMLR, 2018.

[24] Carl Edward Rasmussen. Gaussian processes in machine learning. In *Summer school on machine learning*, pages 63–71. Springer, 2003.

[25] Mark Sandler, Andrew Howard, Menglong Zhu, Andrey Zhmoginov, and Liang-Chieh Chen. Mobilenetv2: Inverted residuals and linear bottlenecks. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 4510–4520, 2018.

[26] Mingxing Tan, Bo Chen, Ruoming Pang, Vijay Vasudevan, Mark Sandler, Andrew Howard, and Quoc V Le. Mnasnet: Platform-aware neural architecture search for mobile. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 2820–2828, 2019.

[27] Joaquin Vanschoren, Jan N. van Rijn, Bernd Bischl, and Luis Torgo. Openml: Networked science in machine learning. *SIGKDD Explorations*, 15(2):49–60, 2013. doi: 10.1145/2641190.2641198. URL http://doi.acm.org/10.1145/2641190.2641198.

[28] Ruoxi Wang, Rakesh Shivanna, Derek Cheng, Sagar Jain, Dong Lin, Lichan Hong, and Ed Chi. Dcn v2: Improved deep & cross network and practical lessons for web-scale learning to rank systems. In *Proceedings of the Web Conference 2021*, pages 1785–1797, 2021.

[29] Colin White, Willie Neiswanger, and Yash Savani. Bananas: Bayesian optimization with neural architectures for neural architecture search. *arXiv preprint arXiv:1910.11858*, 1(2):4, 2019.

[30] Chris Ying, Aaron Klein, Eric Christiansen, Esteban Real, Kevin Murphy, and Frank Hutter. Nasbench-101: Towards reproducible neural architecture search. In *International Conference on Machine Learning*, pages 7105–7114. PMLR, 2019.

[31] Hongpeng Zhou, Minghao Yang, Jun Wang, and Wei Pan. Bayesnas: A bayesian approach for neural architecture search. In *International conference on machine learning*, pages 7603–7613. PMLR, 2019.
A Algorithm Pseudocode

We show pseudocode of the algorithms introduced in Section 3.

Algorithm 1 (Resource-Oblivious) One-Shot Training and REINFORCE

Input: search space $S$, weight learning rate $\alpha$, RL learning rate $\eta$
Output: sampling probabilities $\{p_{ij}\}_{i \in [L], j \in [C_i]}$
1. initialize logits $\ell_{ij} \leftarrow 0$, $\forall i \in [L], j \in [C_i]$
2. initialize quality reward moving average $\hat{Q} \leftarrow 0$
3. layer warmup
4. for $\text{iter} = 1$ to $\max \text{ iter}$ do
5. \hspace{1em} $p_{ij} \leftarrow \exp(\ell_{ij}) / \sum_{j \in [C_i]} \exp(\ell_{ij}), \forall i \in [L], j \in [C_i]$ \hspace{1em} $\triangleright$ weight update
6. \hspace{2em} for $i = 1$ to $L$ do
7. \hspace{3em} $x_i \leftarrow$ the $i$-th layer size sampled from $\{s_{ij}\}_{j \in [C_i]}$ with distribution $\{p_{ij}\}_{j \in [C_i]}$
8. \hspace{3em} $\text{loss}(x) \leftarrow$ the (training) loss of $x = x_1 \cdots x_L$ on the training set
9. \hspace{3em} $w \leftarrow w - \alpha \nabla \text{loss}(x)$, in which $w$ is the weights of $x$ \hspace{.5em} $\triangleright$ can be replaced with optimizers other than SGD
10. \hspace{2em} $\triangleright$ RL update
11. \hspace{2em} for $i = 1$ to $L$
12. \hspace{3em} $y_i \leftarrow$ the $i$-th layer size sampled from $\{s_{ij}\}_{j \in [C_i]}$ with distribution $\{p_{ij}\}_{j \in [C_i]}$
13. \hspace{3em} $Q(y) \leftarrow 1 - \text{loss}(y)$, the quality reward of $y = y_1 \cdots y_L$ on the validation set
14. \hspace{3em} RL reward $r(y) \leftarrow Q(y)$ \hspace{.5em} $\triangleright$ can be replaced with resource-aware rewards introduced in Section 3.3
15. \hspace{3em} $J(y) \leftarrow \text{stop \_ grad}(r(y) - \hat{Q}) \log P(y)$ \hspace{.5em} $\triangleright$ can be replaced with Algorithm 2 when resource-constrained
16. \hspace{3em} $\ell_{ij} \leftarrow \ell_{ij} + \eta \nabla J(y)$, $\forall i \in [L], j \in [C_i]$ \hspace{.5em} $\triangleright$ can be replaced with optimizers other than SGD
17. \hspace{3em} $\hat{Q} \leftarrow \gamma \hat{Q} + (1 - \gamma) \text{Q(y)}$ \hspace{1em} $\triangleright$ update moving average with $\gamma = 0.9$

Algorithm 2 Rejection with Monte-Carlo (MC) Sampling

Input: number of MC samples $N$, feasible set $V$, MC proposal distribution $q$, quality reward moving average $\hat{Q}$, sampled architecture for RL in the current step $y = y_1 \cdots y_L$, current layer size distribution over $\{s_{ij}\}_{j \in [C_i]}$ with probability $\{p_{ij}\}_{j \in [C_i]}$
Output: $J(y)$
1. if $y$ is feasible then
2. \hspace{1em} $Q(y) =$ the quality reward of $y$
3. \hspace{1em} $P(y) := \prod_{i \in [L]} P(Y_i = y_i)$
4. \hspace{2em} for $i = 1$ to $L$ do
5. \hspace{3em} $\{z_{i}^{(k)}\}_{k \in [N]} \leftarrow N$ samples of the $i$-th layer size, sampled from $\{s_{ij}\}_{j \in [C_i]}$ with distribution $\{p_{ij}\}_{j \in [C_i]}$
6. \hspace{3em} $p_{i}^{(k)} := P(Z_i = z_{i}^{(k)}), \forall i \in [L], k \in [N]$
7. \hspace{3em} $P(V) := \prod_{i \in [L]} p_{i}^{(k)}, \forall k \in [N]$
8. \hspace{3em} $\hat{P}(V) \leftarrow \frac{1}{N} \sum_{k \in [N], z^{(k)} \in V} \frac{p_{i}^{(k)}}{P(V)}$, in which $z^{(k)} := z_{1}^{(k)} \cdots z_{L}^{(k)}$
9. \hspace{3em} $J(y) \leftarrow \text{stop \_ grad}(Q(y) - \hat{Q}) \log \frac{P(y)}{\hat{P}(V)}$
10. else
11. \hspace{2em} $J(y) \leftarrow 0$
Figure 10: Illustration of the feasible set $V$ within the search space $S$. Each green diamond or orange dot denotes a feasible or infeasible architecture, respectively.

Algorithm 3 Sample to Return the Final Architecture

1. **Input:** sampling probabilities $\{p_{ij}\}_{i \in [L], j \in [C_i]}$ returned by Algorithm 1, number of desired architectures $n$, number of samples to draw $m$
2. **Output:** the set of $n$ selected architectures $A$
3. for $i = 1$ to $L$ do
4. $\{x^{(k)}_i\}_{k \in [m]} \leftarrow m$ samples of the $i$-th layer size, sampled from $\{s_{ij}\}_{j \in [C_i]}$ with distribution $\{p_{ij}\}_{j \in [C_i]}$
5. $F := \{k \in [m] | x^{(k)}_1 - x^{(k)}_2 - \cdots - x^{(k)}_L \in V\}$
6. $A \leftarrow n$ unique architectures in $F$ with largest numbers of parameters

Notice that in Algorithm 1, we show the weight and RL updates with the stochastic gradient descent (SGD) algorithm; in our experiments on the toy example and real datasets, we use Adam for both updates as in ProxylessNAS \cite{proxylessnas} and TuNAS \cite{tunas}, since it synchronizes convergence across different layer size choices, and slows down the learning which would otherwise converge too rapidly.

B Details of Experiment Setup

B.1 Toy Example

We use the Adam optimizer with $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 0.001$ to update the logits. When we use the Abs Reward, the results are similar when $\eta \geq 0.05$, while the RL controller with $\eta < 0.05$ converges too slow or is hard to converge. When we use the rejection-based reward, we use RL learning rate $\eta = 0.1$; other $\eta$ values with which RL converges give similar results.

B.2 Real Datasets

Table\[1\] shows the datasets we use. Datasets other than Criteo come from the OpenML dataset repository \cite{openml}. For Criteo, we randomly split the labeled part (45,840,617 points) into 90% training (41,258,185 points) and 10% validation (4,582,432 points); for the other datasets, we randomly split into 80% training and 20% validation\[^4^]\[^4^\]. The representations we use for Criteo are inspired by DCN-V2 \cite{dncv2}.

\[^4^\]The ranking of validation losses among architectures under such splits is almost the same as that of test losses under 60%-20%-20% training-validation-test splits.

| name    | # points       | # features | # classes | embedding we use for each feature                          |
|---------|----------------|------------|-----------|------------------------------------------------------------|
|         | # numerical    | # categorical |         |                                                            |
| Criteo  | 51,882,752     | 13         | 26        | original values for each numerical, 39-dimensional for each categorical |
| Volkert | 58,310         | 180        | 0         | original values                                             |
| Aloi    | 108,000        | 128        | 0         | original values                                             |
| Connect-4 | 67,557      | 0          | 42        | 2-dimensional for each categorical                         |
| Higgs   | 98,050         | 28         | 0         | original values                                             |

Table 1: Dataset details
Table 2 shows the hyperparameters we use for stand-alone training and NAS, found by grid search. With these hyperparameters, the best architecture in each of our search spaces (introduced in Appendix B.2.1) has performance that is within ±5% of the best performance in Kadra et al. Table 2, and we achieve these scores with FFNs that only have 5% parameters of the ones there. The Adam optimizer has hyperparameters $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 0.001$. We use layer normalization [3] for all datasets. We use balanced error (weighted average of classification errors across classes) for all other datasets as in Kadra et al., except for Criteo, on which we use logistic loss as in Wang et al.

| name   | batch size | learning rate | learning rate schedule | optimizer              | # training epochs | metric       |
|--------|------------|---------------|------------------------|------------------------|------------------|--------------|
| Criteo | 512        | 0.002         | cosine decay           | Adam                   | 60               | log loss     |
| Volkert| 32         | 0.01          | constant               | SGD with momentum 0.9  | 120              | balanced error |
| Aloi   | 128        | 0.0005        | constant               | Adam                   | 50               | balanced error |
| Connect-4 | 32     | 0.0005       | cosine decay           | Adam                   | 60               | balanced error |
| Higgs  | 64         | 0.05          | constant               | SGD                    | 60               | balanced error |

We use constant RL learning rates for NAS. The Connect-4 and Higgs datasets are easy for both the Abs Reward and rejection-based reward, in the sense that small FFNs with fewer than 5,000 parameters can achieve near-SOTA results (±5% of the best accuracy scores listed in Kadra et al. Table 2, except that we do 80%-20% training-validation splits and use original instead of standardized features), and RL-based weight-sharing NAS with either reward can find architectures that match the Pareto-optimal reference architectures. The Aloi dataset needs more parameters (more than 100k), but the other observations are similar to on Connect-4 and Higgs. Thus we omit the corresponding results.

The factorized search spaces we use for NAS are:

- Criteo: Each layer has 20 choices {8, 16, 24, 32, 48, 64, 80, 96, 112, 128, 144, 160, 176, 192, 208, 224, 240, 256, 384, 512}.
- Volkert, 4-layer networks: Each layer has 20 choices {8, 16, 24, 32, 48, 64, 80, 96, 112, 128, 144, 160, 176, 192, 208, 224, 240, 256, 384, 512}.
- Volkert, 9-layer networks: Each layer has 12 choices {8, 16, 24, 32, 48, 64, 80, 96, 112, 128, 144, 160}.

This search space has fewer choices for each hidden layer than the 4-layer counterpart, but the size of the search space is over $3 \times 10^4$ times larger.

### B.2.1 More Details on the Tradeoff Plot (Figure 3)

Each search space we use for exhaustive search and NAS has a fixed number of hidden layers. Resource-constrained NAS in a search space with varying number of hidden layers is an interesting problem for future studies. On each dataset, we randomly sample, train and evaluate architectures in the search space with the number of parameters fall within a range, in which there is a clear tradeoff between loss and number of parameters. These ranges are:

- Criteo: 0 – 200,000
- Volkert, 4-layer networks: 15,000 – 50,000
- Volkert, 9-layer networks: 40,000 – 100,000

The performance ranking of architectures under the balanced error metric is almost the same as under logistic loss. Also, the balanced error metric is only for reporting the final validation losses; both weight and RL updates use logistic loss.

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5 The performance ranking of architectures under the balanced error metric is almost the same as under logistic loss. Also, the balanced error metric is only for reporting the final validation losses; both weight and RL updates use logistic loss.

6 https://www.openml.org/d/41669

7 https://www.openml.org/d/23512

8 https://www.openml.org/d/42396
Figure 11: Tradeoffs between validation loss and number of parameters in four search spaces.

Figure 11 shows the tradeoffs between loss and number of parameters in these search spaces. When training each architecture 5 times, the standard deviation (std) across different runs is 0.0002 for Criteo and 0.004 for Volkert, meaning that the architectures whose performance difference is larger than $2 \times \text{std}$ are qualitatively different with high probability. We use Pareto-optimal architectures as the reference of resource-constrained NAS: we want an architecture that both matches (or even beats) the performance of the reference architecture and has no more parameters than the reference. Most Pareto-optimal architectures in Figure 11 have the bottleneck structure; Table 3 shows some examples.

B.2.2 More Details on TPU Implementation

When we run one-shot NAS on a TPU that has multiple TPU cores (for example, each Cloud TPU-v2 we use has 8 cores), each core samples an architectures independently, and we use the average loss and reward for weight and RL updates, respectively. This means our algorithm actually samples multiple architectures in each iteration and uses the `tensorflow.tpu.cross_replica_sum()` method to compute their average effect on the gradient. Since only a fraction of architectures are feasible in each search space, we set the losses and rewards given by the infeasible architectures to 0 before averaging, so that we are equivalently only averaging across the sampled architectures that are feasible. We then reweight the average loss or reward with $\frac{\text{number of cores}}{\text{number of feasible architectures}}$ to obtain an unbiased estimate.

B.2.3 More Details on the NAS Method Comparison Plot (Figure 2)

For each architecture below, we report its number of parameters and mean $\pm$ std logistic loss across 5 stand-alone training runs in brackets.

We have the reference architecture 32-144-24 (41,153 parameters, 0.4454 $\pm$ 0.0003) for NAS methods to match. In the search space with $20^3 = 8000$ candidate architectures:

- TabNAS trials with no fewer than 2,048 Monte-Carlo samples and the RL learning rate $\eta$ among {0.001, 0.005, 0.01} consistently finds either the reference architecture itself, or an architectures that

---

Note that the Pareto optimality of the reference architecture is determined by only one round of random search. Thus because of the randomness across multiple training runs, the other architectures are likely to beat the reference architecture: a “regression toward the mean”.

---
Table 3: Some Pareto-optimal architectures in Figure 11. All architectures shown here and almost all other Pareto-optimal architectures have the bottleneck structure.

| Search space | Pareto-optimal architecture | Number of parameters | Loss  
|-------------|----------------------------|----------------------|-----|
| Figure 11(a) | Criteo 4-layer 32-144-24-112 | 44,041 | 0.4454 |
| Figure 11(a) | Criteo 4-layer 48-112-8-80 | 56,537 | 0.4448 |
| Figure 11(a) | Criteo 4-layer 48-384-16-176 | 77,489 | 0.4441 |
| Figure 11(a) | Criteo 4-layer 96-144-32-240 | 125,457 | 0.4433 |
| Figure 11(a) | Criteo 4-layer 96-384-48-16 | 155,217 | 0.4430 |
| Figure 11(b) | Criteo 5-layer 32-240-16-8-96 | 45,769 | 0.4451 |
| Figure 11(b) | Criteo 5-layer 48-128-64-16-128 | 67,217 | 0.4446 |
| Figure 11(b) | Criteo 5-layer 48-256-16-8-384 | 69,977 | 0.4443 |
| Figure 11(b) | Criteo 5-layer 64-144-48-96-160 | 102,497 | 0.4437 |
| Figure 11(b) | Criteo 5-layer 96-512-24-256-48 | 179,449 | 0.4430 |
| Figure 11(c) | Volkert 4-layer 48-112-16-24 | 16,642 | 0.3314 |
| Figure 11(c) | Volkert 4-layer 32-112-24-224 | 20,050 | 0.3269 |
| Figure 11(c) | Volkert 4-layer 48-160-32-144 | 27,882 | 0.3149 |
| Figure 11(c) | Volkert 4-layer 48-256-24-112 | 31,330 | 0.3097 |
| Figure 11(c) | Volkert 4-layer 80-208-32-64 | 40,778 | 0.3054 |
| Figure 11(d) | Volkert 9-layer 64-64-160-48-144-16-8-48 | 40,482 | 0.3250 |
| Figure 11(d) | Volkert 9-layer 80-144-32-112-32-8-128-8-144 | 43,290 | 0.3238 |
| Figure 11(d) | Volkert 9-layer 112-144-32-24-24-24-128-32 | 51,890 | 0.3128 |
| Figure 11(d) | Volkert 9-layer 144-128-112-16-16-48-144-24-160 | 78,114 | 0.3019 |
| Figure 11(d) | Volkert 9-layer 160-144-44-32-112-32-48-32-144 | 94,330 | 0.3010 |

is qualitatively the same as the reference, like 32-112-32 (40,241 parameters, 0.4456 ± 0.0003).

- NAS with the Abs Reward: After grid search over RL learning rate $\eta$ (among {0.0001, 0.0005, 0.001, 0.005, 0.01, 0.015, 0.02, 0.025, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.1, 0.15, 0.2, 0.25, 0.3, 0.4, 0.5, 0.75, 1.0, 1.5, 2.0}) and $\beta$ (among {-0.0005, -0.001, -0.005, -0.01, -0.05, -0.1, -0.5, -0.75, -1.0, -1.25, -1.5, -2.0, -3.0}), the RL controller finds 32-64-96 (41,345 parameters, 0.4461 ± 0.0003) or 32-80-64 (40,785 parameters, 0.4459 ± 0.0002) among over 90% trials that eventually find an architecture within ±5% of the target number of parameters 41,153.

### B.3 Difficulty in Using the MnasNet Reward

With the MnasNet reward, only fewer than 1% NAS trials in our hyperparameter grid search (the ones with a medium $\beta$) can find an architecture whose number of parameters is within ±5% of the reference, and among which none or only one (out of tens) can match the reference performance. In contrast, TuNAS with the Abs Reward finds an architecture with number of parameters within ±5% of the reference among over 50% of the grid search trials described in Appendix B.2.3 and TabNAS with the rejection-based reward consistently finds such architectures at medium RL learning rates $\eta$ and decently large numbers of MC samples $N$. This means it is significantly more difficult to use the MnasNet reward than competing approaches in the practice of resource-constrained tabular NAS.

### C More Failure Cases of the Abs Reward

For each architecture below, we report its number of parameters and mean ± std loss across 5 stand-alone training runs (logistic loss for Criteo, balanced error for the others) in brackets.

**On Criteo, in the 4-layer search space.** We have the reference architecture 48-128-16-112 (59,697 parameters, 0.4451 ± 0.0002) for NAS to match in the search space (shown as Figure 11(a)). Similar to...
Figure 2 we show similar results on NAS with rejection-based reward (TabNAS) and NAS with the Abs Reward (TuNAS) in Figure 12(a). In the search space with $20^4 = 1.6 \times 10^5$ candidate architectures:

- TabNAS with 32,768 Monte-Carlo samples and RL learning rate $\eta$ among $\{0.001, 0.005, 0.01\}$ consistently finds architectures qualitatively the same as the reference. Example results include 48-128-24-32 (59,545 parameters, 0.4449 ± 0.0002), 48-144-16-48 (59,585 parameters, 0.4448 ± 0.0001), 48-112-16-144 (59,233 parameters, 0.4448 ± 0.0002) and the reference architecture itself.
- NAS with the Abs Reward successfully finds the reference architecture 48-128-16-112 in 3 out of 338 hyperparameter settings on a $\beta$-$\eta$ grid. Other found architectures include 48-80-32-112 (59,665 parameters, 0.4452 ± 0.0002), 32-128-80-144 (59,249 parameters, 0.4453 ± 0.0003) and 48-160-8-48 (58,953 parameters, 0.4448 ± 0.0003), among which the first two are inferior to the TabNAS-found counterparts.

On Criteo, in the 5-layer search space. We have the reference architecture 48-240-24-256-8 (75,353 parameters, 0.4448 ± 0.0002) for NAS methods to match in the search space (shown as Figure 11(b)). Similar to Figure 2 we have similar results on the comparison among random sampling, NAS with rejection-based reward (TabNAS), and NAS with the Abs Reward as Figure 12(b). In the search space with $20^5 = 3.2 \times 10^6$ candidate architectures:

- TabNAS with 32,768 Monte-Carlo samples and the RL learning rate $\eta = 0.005$ consistently finds architectures qualitatively the same as the reference. Example results include 48-176-64-16-256 (74,945 parameters, 0.4445 ± 0.0002), 48-208-48-48-64 (75,121 parameters, 0.4444 ± 0.0001), 48-256-32-80-24 (74,721 parameters, 0.4446 ± 0.0003) and 48-180-80-16-96 (75,153 parameters, 0.4445 ± 0.0002).
- NAS with the Abs Reward finds 64-80-48-24 (27,658 parameters, 0.3305 ± 0.0038), 64-96-8-32-64 (75,273 parameters, 0.4445 ± 0.0001) that are mostly inferior to the TabNAS-found architectures.

On Volkert, in the 4-layer search space. We have the reference architecture 48-160-32-144 (27,882 parameters, 0.3244 ± 0.0040) for NAS to match in the search space (shown as Figure 11(c)). Similar to Figure 2 we draw the comparison plot among random sampling, NAS with rejection-based reward (TabNAS), and NAS with the Abs Reward as Figure 12(c). In the search space with $1.6 \times 10^5$ candidate architectures:

- TabNAS with $1 \times 10^4$ Monte-Carlo samples and the RL learning rate $\eta \in \{0.001, 0.005, 0.01, 0.05\}$ consistently finds either the reference architecture itself or other architectures qualitatively the same. Examples include 64-128-48-16 (27,050 parameters, 0.3237 ± 0.0040), 80-48-112-32 (27,802 parameters, 0.3274 ± 0.0037), 64-96-80-24 (27,778 parameters, 0.3279 ± 0.0005), and 64-144-32-48 (27,658 parameters, 0.3204 ± 0.0038).
- NAS with the Abs Reward finds 96-64-32-48 (27,738 parameters, 0.3302 ± 0.0042), 96-48-32-96 (27,738 parameters, 0.3305 ± 0.0047), 64-80-16-48 (27,738 parameters, 0.3302 ± 0.0050), 112-48-24-24 (27,722 parameters, 0.3301 ± 0.0034) and 80-80-48-48 (27,690 parameters, 0.3309 ± 0.0022) that are inferior.

On Volkert, in the 9-layer search space. We further do NAS on Volkert in the 9-layer search space to test the ability of TabNAS in searching among significantly deeper FFNs. The tradeoff between loss and number of parameters in the search space is shown in Figure 11(d). We have the reference architecture 144-128-112-16-16-48-144-24-160 (78,114 parameters, 0.3126 ± 0.0050) for NAS to match. We compare random sampling, NAS with rejection-based reward (TabNAS), and NAS with the Abs Reward in Figure 12(d). In the search space with $5.2 \times 10^9$ candidate architectures (which is nearly impossible for exhaustive search):

- TabNAS with $5 \times 10^6$ Monte-Carlo samples and the RL learning rate $\eta \in \{0.002, 0.005\}$ consistently finds architectures that are qualitatively the same as the reference. These architectures are found when the RL controller is far from converged and when $P(V)$ slightly decreases after RL starts. Example results include 144-144-112-64-24-16-128-8-128 (78,026 parameters, 0.3120 ± 0.0049), 128-160-96-32-24-64-64-32-160 (77,890 parameters, 0.3127 ± 0.0040), 128-144-112-32-64-64-80-16-128
Figure 12: Rejection-based reward distributionally outperforms random search and resource-aware Abs Reward in a number of search spaces. The points and error bars have the same meaning as in Figure 2. The time taken for each stand-alone training run (the unit length for x axes) is 2.5 hours on Criteo (Figure 12(a) and 12(b)), 10 minutes on Volkert with 4-layer FFNs (Figure 12(c)), and 22-25 minutes on Volkert with 9-layer FFNs (Figure 12(d)).

As a side note, previous works like MnasNet and TuNAS (often or only on vision tasks) do often have inverted bottleneck blocks in their search spaces. However, the search spaces used there have a hard-coded requirement that certain layers must have bottlenecks. In contrast, our search spaces permit the controller to automatically determine whether to use bottleneck structures based on the task under consideration. This is important because networks with bottlenecks do not always outperform others on all tasks. For example, the reference architecture 32-144-24 outperforms the TuNAS-found 32-64-96 on Criteo, but the reference 64-192-48-32 (64,568 parameters, 0.0662 ± 0.0011) is on par with the TuNAS-and-TabNAS-found 96-80-96-32 (64,024 parameters, 0.0669 ± 0.0013) on Aloi.
Table 4: Comparison of TabNAS, Bayesian optimization (BO) and evolutionary search (ES) with weight sharing. TabNAS finds the architecture with the smallest loss.

| method          | found architecture (number of parameters, mean ± std loss)          |
|-----------------|---------------------------------------------------------------------|
| TabNAS (N=32,768) | 48-176-64-16-256 (74,945 parameters, 0.4445 ± 0.0002)               |
| BO (RBF kernel L=10) | 64-80-8-16-16 (72,073 parameters, 0.4447 ± 0.0002)                |
| BO (RBF kernel L=1)   | 48-80-48-96-96 (71,265 parameters, 0.4451 ± 0.0003)               |
| ES (10 steps, population 100) | 48-96-16-144-64 (67,393 parameters, 0.4450 ± 0.0002)             |
| ES (60 steps, population 50) | 48-48-80-80-64 (67,345 parameters, 0.4452 ± 0.0003)              |

D Comparison with Weight-Sharing Bayesian Optimization and Evolutionary Search

Bayesian optimization (BO) and evolutionary search (ES) are popular strategies for NAS (see e.g., [12, 15, 29, 31]; [19, 2]). We are not aware of any work that successfully applies BO or ES for weight-sharing NAS. Thus we design the following (novel) methods of BO or ES for weight-sharing NAS: train the SuperNet for the same number of epochs as RL, and then do BO (by Gaussian processes [24] with expected improvement [21, 13]) or ES in the set of feasible architectures with the SuperNet one-shot losses (evaluated from SuperNet weights). These methods omit the extra forward passes for RL controller training, but need extra forward passes to evaluate child networks. We control the number of passes for a fair comparison. On Criteo, the cost of forward passes for RL is comparable to evaluating 405 child networks, and the search space of 5-layer FFNs has 340,590 feasible architectures below the 75,353 parameters limit in Figure 11(b). The corresponding reference architecture is 48-240-24-256-8. The architectures found by BO and ES (under multiple hyperparameter settings) are sensitive to initialization and are worse (see Table 4). Thus RL explores the search space more efficiently than BO and ES: it finds the global optimum with fewer forward passes.

E Difficulty of Hyperparameter Tuning

Hyperparameter tuning has always been a headache for machine learning. In the design of NAS approaches, the hope is that the NAS hyperparameters are much easier to tune than the architectures NAS search over. We denote the RL learning rate and the number of MC samples by $\eta$ and $N$, respectively. The three resource-aware rewards (in MnasNet and TuNAS) have both $\eta$ and $\beta$ as hyperparameters; our TabNAS with the rejection-based reward has $\eta$ and $N$ to tune.
### E.1 Resource Hyperparameter $\beta$

$\beta$ is difficult to tune in experiments: the best value varies by dataset and lies in the middle of its search space. Since $\beta < 0$, we discuss its absolute value. In a NAS search space, the architecture that is feasible and can match the reference performance often has the number of parameters that is more than 98% of the reference. A too small $|\beta|$ is not powerful enough to enforce the resource constraint, in which case NAS finds an architecture that is far from the target number of parameters and makes the search nearly unconstrained (e.g., the Abs Reward with $|\beta| = 1$ in the toy example, shown in Figure 1, and towards the left end in Figure 13(a)). A too large $|\beta|$ severely penalizes the violation of the resource constraint, in which case the RL controller would always give an architecture close to the reference, with much bias (e.g., the Abs Reward with $|\beta| = 2$ in Figure 1, and towards the right end in Figure 13(a)). Thus practitioners seek a medium $|\beta|$ in hyperparameter tuning to both obey the resource constraint and achieve a better result. In our experiments, such “appropriate” medium values vary largely across datasets: 1 on Criteo with the 32-144-24 reference architecture (41,153 parameters), 2 on Volkert with the 48-160-32-144 reference architecture (27,882 parameters), and 25 on Aloi with the 64-192-48-32 reference architecture (64,568 parameters).

### E.2 RL Learning Rate $\eta$

The RL learning rate $\eta$ is easier to tune and more generalizable across datasets than $\beta$. With a large $\eta$, the RL controller quickly converges right after the first 25% epochs of layer warmup; with a small $\eta$, the RL controller converges slowly or may not converge, although there may still be enough signal from the layerwise probabilities to get the final result. It is thus straightforward to tune $\eta$ by observing the convergence behavior of sampling probabilities. In our experiments, the appropriate value of $\eta$ does not significantly vary across tasks: a constant $\eta \in [0.001, 0.01]$ is appropriate for all datasets and all number of parameter limits.

### E.3 Number of MC Samples $N$

The number of MC samples $N$ is also easier to tune than $\beta$. Resource permitting, $N$ is the larger, the better (Figure 13(b)), so that $P(V)$ can be better estimated. When $N$ is too small, the MC sampling has a high chance of missing the valid architectures in the search space, and thus incurs large bias and variance for the estimate of $\nabla \log[P(y | y \in V)]$. In such cases, $\hat{P}(V)$ may miss all valid architectures at the beginning of RL and quickly converge to 0. $\hat{P}(V)$ being equal or close to 0 is a bad case for our rejection-based algorithm: the single-step RL objective $J(y)$ that has a $- \log(\hat{P}(V))$ term grows extremely large and gives an explosive gradient to stuck the RL controller in the current choice. Consequently, the criterion for choosing $N$ is to choose the largest that can afford, and hopefully, at least choose the smallest that can make $\hat{P}(V)$ steadily increase during RL. Figure 14 shows the changes of $\hat{P}(V)$ on Criteo with the 32-144-24 reference in the search space of 8,000 architectures at three $N$ values. The NAS succeeds when $N \geq 2048$, same as the threshold that makes $\hat{P}(V)$ increase.

Overall, the RL controller with our rejection-based reward has hyperparameters that are easier to tune than with resource-aware rewards in MnasNet and TuNAS.

### F  More on Ablation with a Non-Differentiable $P(V)$ (or $\hat{P}(V)$)

As discussed in Section 4.3, the found architectures are significantly worse when $P(V)$ is omitted from $J(y)$. Below are our experimental findings:

- In the case that we do not skip infeasible architectures in weight updates, the largest hidden layer sizes may gain and maintain the largest sampling probabilities soon after RL starts. This is because most architectures in the 3-layer Criteo search space are above the number of parameters limit 41,153. When RL starts, the sampled feasible architectures underperform the moving average, thus their logits are severely penalized, making the logits of the infeasible architectures (which often have wide hidden layers) quickly dominate (Figure 15(a)). Accordingly, the (estimated) valid probability $P(V)$
(or \(\hat{P}(V)\)) quickly decrease to 0 (Figure 15(b)), and the RL controller gets stuck (as described in Appendix [E.3] in these large choices for hidden layer sizes.

- In the case that we skip infeasible architectures in both weight and RL updates, the RL controller eventually picks feasible architectures with bottleneck structures, but the found architectures are almost always suboptimal: when RL starts, the controller severely boosts the logits of the sampled feasible architectures without much exploration in the search space, and quickly gets stuck there. For example, the search in Figure 15(c) finds 24-384-16 (40,449 parameters) that is feasible but suboptimal: \(P(V)\) and \(\hat{P}(V)\) quickly increase to 1 after RL starts (Figure 15(d)).

**Figure 15:** Failure cases in ablation when \(\hat{P}(V)\) is non-differentiable. We show results with RL learning rate \(\eta = 0.005\); those under other \(\eta\) values are similar.

### G  Proofs

#### G.1 \(\hat{P}(V)\) is an Unbiased and Consistent Estimate of \(P(V)\)

Within the search space \(S\), recall the definitions of \(P(V)\) and \(\hat{P}(V)\):

- \(P(V) = \sum_{z^{(i)} \in S} p^{(i)} \mathbb{1}(z^{(i)} \in V)\)
- \(\hat{P}(V) = \frac{1}{N} \sum_{k \in [N], z^{(k)} \in V} q^{(k)} = \frac{1}{N} \sum_{k \in [N]} \hat{E}^{(k)} \mathbb{1}(z^{(k)} \in V)\)

**Unbiasedness.** With \(N\) architectures sampled from the proposal distribution \(q\), we take the expectation with respect to \(N\) sampled architectures:

\[
E[\hat{P}(V)] = \frac{1}{N} \mathbb{E} \left[ \sum_{k \in [N], z^{(k)} \in V} \frac{p^{(k)}}{q^{(k)}} \right]
= \frac{1}{N} \mathbb{E} \left[ \sum_{k \in [N]} \frac{p^{(k)}}{q^{(k)}} \mathbb{1}(z^{(k)} \in V) \right]
= \frac{1}{N} \sum_{k \in [N]} \mathbb{E} \left[ \frac{p^{(k)}}{q^{(k)}} \mathbb{1}(z^{(k)} \in V) \right],
\]

in which each summand

\[
\mathbb{E} \left[ \frac{p^{(k)}}{q^{(k)}} \mathbb{1}(z^{(k)} \in V) \right] = \sum_{z^{(i)} \in S} q^{(k)} \frac{p^{(k)}}{q^{(k)}} \mathbb{1}(z^{(k)} \in V)
= P(V),
\]

Thus \(E[\hat{P}(V)] = P(V)\).
Thus we have
\[ \text{Var}[\hat{P}(V)] = \frac{1}{N} \sum_{k \in [N]} \text{Var} \left[ \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V) \right], \]
in which each summand
\[ \text{Var} \left[ \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V) \right] = \mathbb{E} \left[ \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V) - P(V) \right]^2 \]
\[ = \sum_{z(k) \not\in V} q(k)P(V)^2 + \sum_{z(k) \in V} q(k) \left[ \frac{p(k)}{q(k)} - P(V) \right]^2 \]
\[ = -P(V)^2 + \sum_{z(k) \in V} \left( \frac{p(k)}{q(k)} \right)^2, \]
thus the variance
\[ \text{Var}[\hat{P}(V)] = \frac{1}{N} \sum_{k \in [N]} \text{Var} \left[ \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V) \right] \]
\[ = \frac{1}{N} \left[ -P(V)^2 + \sum_{z(k) \in V} \left( \frac{p(k)}{q(k)} \right)^2 \right], \]
which goes to 0 as \( N \to \infty \). It worths noting that when we set \( q = \text{stop\_grad}(p) \), the single-summand variance (Equation 1) becomes \( P(V) - P(V)^2 \), which is the variance of a Bernoulli distribution with mean \( P(V) \).

The Chebyshev’s Inequality states that for a random variable \( X \) with expectation \( \mu \), for any \( a > 0 \), \( P(|X - \mu| > a) \leq \frac{\text{Var}(X)}{a^2} \). Thus \( \lim_{N \to \infty} \text{Var}(X) = 0 \) implies that \( \lim_{N \to \infty} P(|X - \mu| > a) = 0 \) for any \( a > 0 \), indicating consistency.

**Consistency.** We first show the variance of \( P(V) \) converges to 0 as the number of MC samples \( N \to \infty \).

Because of independence among samples,
\[ \text{Var}[\hat{P}(V)] = \frac{1}{N} \sum_{k \in [N]} \text{Var} \left[ \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V) \right], \]

G.2 \( \nabla \log[\hat{P}(V)] \) is a Consistent Estimate of \( \nabla \log[P(y \mid y \in V)] \)

Since \( P(y \mid y \in V) = \frac{P(y)}{P(V)} \), we show \( \text{plim}_{N \to \infty} \nabla \log \hat{P}(V) = \nabla \log P(V) \) below to prove consistency, in which \( \text{plim} \) denotes convergence in probability.

Recall \( p^{(i)} \) is the probability of sampling the \( i \)-th architecture \( z^{(i)} \) within the search space \( S \), and the definitions of \( P(V) \) and \( \hat{P}(V) \) are:

- \( P(V) = \sum_{z^{(i)} \in S} p^{(i)} \mathbb{1}(z^{(i)} \in V) \),
- \( \hat{P}(V) = \frac{1}{N} \sum_{k \in [N], z^{(i)} \in V} \frac{p(k)}{q(k)} = \frac{1}{N} \sum_{k \in [N]} \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V) \), in which each \( p(k) \) is differentiable with respect to all logits \( \ell_{ij} \) \( i \in [L], j \in [C] \).

Thus we have
\[ \text{plim}_{N \to \infty} \hat{P}(V) = \text{plim}_{N \to \infty} \frac{1}{N} \sum_{k \in [N]} \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V) \]
\[ = \frac{1}{N} \sum_{z^{(k)} \in S} \frac{p(k)}{q(k)} \mathbb{1}(z(k) \in V)Nq^{(k)} \]
\[ = \sum_{z^{(k)} \in S} p^{(k)} \mathbb{1}(z^{(k)} \in V) = P(V), \]
and
\[
\text{plim}_{N \to \infty} \nabla \hat{P}(V) = \text{plim}_{N \to \infty} \frac{1}{N} \sum_{k \in [N]} \frac{\nabla p^{(k)}}{q^{(k)}} \mathbf{1}(z^{(k)} \in V)
\]
\[
= \frac{1}{N} \sum_{z^{(k)} \in S} \frac{\nabla p^{(k)}}{q^{(k)}} \mathbf{1}(z^{(k)} \in V) N q^{(k)}
\]
\[
= \sum_{z^{(k)} \in S} \nabla p^{(k)} \mathbf{1}(z^{(k)} \in V) = \nabla P(V).
\]

Together with the condition that $P(V) > 0$ (the search space contains at least one feasible architecture), we have the desired result for consistency as
\[
\text{plim}_{N \to \infty} \nabla \log \hat{P}(V) = \text{plim}_{N \to \infty} \frac{\nabla \hat{P}(V)}{P(V)} = \frac{\text{plim}_{N \to \infty} \nabla \hat{P}(V)}{\text{plim}_{N \to \infty} P(V)} = \nabla \log P(V),
\]
in which the equalities hold due to the properties of convergence in probability.