Understanding and Optimizing Packed Neural Network Training for Hyper-Parameter Tuning

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Abstract
As neural networks are increasingly employed in machine learning practice, organizations will have to determine how to share limited training resources among a diverse set of model training tasks. This paper studies jointly training multiple neural network models on a single GPU. We present an empirical study of this operation, called pack, and end-to-end experiments that suggest significant improvements for hyperparameter search systems. Our research prototype is in TensorFlow, and we evaluate performance across different models (ResNet, MobileNet, DenseNet, and MLP) and training scenarios. The results suggest: (1) packing two models can bring up to 40% performance improvement over unpacked setups for a single training step and the improvement increases when packing more models; (2) the benefit of a pack primitive largely depends on a number of factors including memory capacity, chip architecture, neural network structure, and batch size; (3) there exists a trade-off between packing and unpacking when training multiple neural network models on limited resources; (4) a pack-based Hyperband is up to 2.7× faster than the original Hyperband training method in our experiment setting, with this improvement growing as memory size increases and subsequently the density of models packed.

1 Introduction
The successes of modern AI are in part due to the adoption of neural network models which can place immense demand on computing infrastructure. It is increasingly the case that a diverse set of model training tasks share limited training resources. The long-running nature of these tasks and the large variation in their size and complexity makes efficient resource sharing a crucial concern. Concerns are compounded by an extensive trial-and-error development process where parameters are tuned and architectures are tweaked that result in a large number of trial models to train. Beyond the monetary and resource costs, there are long-term questions of economic and environmental sustainability of this methodology [31, 34].

Efficiently sharing the same infrastructure among multiple training tasks, or multi-tenant training, is proposed to address the issue [13, 24, 25, 38]. The role of a multi-tenancy framework is to stipulate policies and constraints on how contended resources are partitioned and tasks are placed on physical hardware. Most existing approaches divide resources at the granularity of full devices (e.g., an entire GPU) [9]. Such a policy can result in poor resource utilization due to its coarse granularity. For example, models may greatly vary in size, where the largest computer vision models require multiple GBs of GPU memory [2] but mobile-optimized networks use a significantly smaller space [30]. Given that GPUs today have significantly more on-board memory than in the past (e.g., up-to 32 GB in commercial offerings), if a training workload consists of a large number of small neural networks, allocating entire devices to these training tasks is wasteful and significantly delays any large model training.

Furthermore, the reliance of specialized hardware such as GPUs makes fine-grained resource sharing (i.e., training multiple networks on the same device) significantly harder than the typical examples in cloud systems. Unlike CPUs, the full virtualization of GPU resources is very nascent [27]. While modern GPU libraries support running multiple execution kernels in parallel, sharing resources using isolated kernels is an inefficient solution in this setting. Many deep learning workloads are highly redundant, for example, the typical parameter tuning process trains the same model on the same data with small changes in hyperparameters or network architectures. In this setting, those parallel kernels would transfer and store multiple copies of the same training data on the device. This is analogous to the redundancy problems faced with conventional hypervisors running many copies of the same operating system on a single physical server [36].

To avoid these pitfalls and provide efficient sharing, we need an approach that is aware of common I/O and compute processes among models that share a device. We consider a scheme, pack models, where multiple static neural network architectures (e.g., ones that are typically used in Computer Vision) can be rewritten as a single concatenated network that
preserves the input, output, and backpropagation semantics. Not only does such concatenation facilitate partitioning of a single device it also allows us to synchronize data processing threads on GPUs and collapse common variables in the computation graph. It is often the case during hyperparameter or neural architecture search that multiple similar networks are trained, and packed configurations can feed a single I/O stream of training examples to each variant of the network. In contrast, an isolated sharing configuration may lead to duplicated work and wasted resources.

One of the surprising conclusions of this paper is that packing models together is not strictly beneficial. Counter-intuitively, certain packing policies can perform significantly worse than whole-device baselines—other words training a packed model can be slower than the sum of its parts. These effects are particularly significant on GPUs, where results suggest that packing models that are too different can result in excessive blocking and wasted work. In light of these results, this paper studies the range of possible improvements (and/or overheads) for using packed configurations. Further, we design an algorithm that heuristically finds performant packing configurations, and demonstrate that such an algorithm can greatly improve the performance of hyperparameter tuning tasks in terms of the time needed to find the best model.

Our experimental results suggest: (1) There is a range of performance impact, spanning from 40% faster execution to 10% slower execution on a single GPU for packing two models over unpacking them for a single training step, and the improvement is scalable when packing more models. (2) Benefits of a pack primitive largely depend on a number of factors including memory capacity, chip architecture, neural network structure, batch size, and data preprocessing overlap. For example, if the models that are packed together are too different, the synchronized parallelism in GPU execution can lead to excessive blocking. (3) There exists a trade-off between packing and unpacking when training multiple neural network models on limited resources. This trade-off is further complicated by architectural properties that might make a single training step bounded by computation (e.g., backpropagation is expensive) or data transferring (e.g., transferring training batches to GPU memory). (4) The pack primitive can speedup hyperparameter tuning tasks by up to 2.7×.

2 Background

First, we motivate the pack primitive and discuss its basic functioning.

2.1 Motivation

Figure 1 illustrates the typical data flow in neural network model training with stochastic gradient descent (or related optimization algorithms). Consider the typical training setup on the left side. We use the term "host" to describe CPU/Main-Memory/Disk hierarchy and "device" to refer to the GPU/GPU Memory. In this setup, all of the training data resides on the host. In each training step, a sample of data is taken from the host and copied to the device (Figure 1 phase 1). Additionally, it is common in image processing that this data is randomly transformed before it is copied over. These transformations help the neural network generalize to different types of images (Figure 1 phase 2). Then, on the device, the execution framework calculates a gradient using backpropagation (Figure 1 phase 3). Finally, using the results from the backpropagation, the model is updated (Figure 1 phase 4).

In the typical one model-one device configuration, the only option for resource sharing is temporal—where one training task uses the whole GPU first and then switches full control to another task. This configuration is wasteful if the models are small and there is sufficient GPU memory to fit both models on the device simultaneously. The right side of Figure 1 motivates a different solution. This packed configuration also has an added benefit. Suppose, we are training two models on the same dataset to test if a small tweak in network architecture will improve performance. The same data would have to be copied to each GPU, and if they are sharing a PCI-E bus this extra work could significantly hurt performance if enough data is transferred. If the system could pack together models when compatible in size, then these redundant data streams can be fused together to improve performance.
2.2 Basic Framework API

We desire a framework that can pack models together when possible and jointly optimize their respective computation graphs to reduce redundant work. Our current implementation is on top of TensorFlow, but the ideas are generally compatible with other libraries and platforms. We assume that we have access to a full neural network description, as well as the weights of the network. Each model instance has a logical name that uniquely identifies it in the whole system (e.g., "resnet-031219"), and our training system consists of named devices (e.g., ‘gpu:1’). Each training task is identified by four inputs.

- **Model.** A computation graph description of the model to train specified in TensorFlow with pointers to the input and output variables.

- **Optimizer.** A SGD-like optimization algorithm with references to the differentiation and parameter-update operations.

- **Batch Size.** The batch size used in the optimization algorithm, where each batch refers to the size of input data used in a single optimizer step.

- **Steps.** The number of steps to train the model, which is also relevant to the number of epochs since typically one epoch consists of numerous steps.

Our objective is the following isolation guarantee: given these four inputs, our framework will train the models in a fine-grained way but preserve the accuracy as if the training tasks were trained sequentially on a dedicated device. No action that the system takes should affect training accuracy. Such a system requires three basic primitives **load**, **pack**, and **free**. Users should be able to interact with our future system without worrying about exactly how the resources are allocated and on which devices the models are placed.

The primitives **load** and **free** can copy in and copy out models. Given a device name and model id, **load** places the model on the device:

```python
load(model, device)
```

Given a device name and model id, **free** retrieves the model and frees the resources taken by the model on the device:

```python
checkpoint = free(model, device)
```

State-of-the-art neural network training algorithms have additional state as a part of the optimizer. This state is negligible in size and is simply stored with the model.

Then, the API provides the packing primitive **pack**. Suppose, we have two neural networks:

```python
output1 = nn1(input1)
output2 = nn2(input2)
```

The **pack** primitive combines both models into a new neural network by concatenating the output layers:

```python
[output1 output2] = nn12([input1, input2])
```

This **pack** operation is fully differentiable and preserves the correctness semantics of the two original networks. Crucially this allows the execution layer to process inputs simultaneously.

Thus, in a packed configuration, the models can be jointly trained. The training steps have to be synchronized in the sense that the models are differentiated and updated at the same time. This synchronization leads to a complex performance tradeoff—i.e., the models are too different the device may waste effort stalling on one model while either updating or differentiating on the other. This means that a packed configuration may be significantly slower than sequentially training each model. However, the overheads from stalling may be counteracted by the benefits of reducing redundant computation. Navigating this complex tradeoff space is the motivation for this study, and we seek to understand under what conditions is packing beneficial.

3 Implementation

We build a prototype system on top of TensorFlow with image classification as our motivating application in our implementation. However, our implementation is general-purpose and can support various models for different applications.

3.1 Basic Packing

Packing is a lossless operation that simply concatenates the outputs of two or more neural networks. Since it is lossless, it preserves the forward and backward pass semantics of the model. The basic operation can be written as stacking two output variables:
resnet_out = ... #reference to resnet output
mobilenet_out = ..#reference to mobilenet output
packed_output = stack([resnet_out, mobilenet_out])

This packed_output can be thought of as a new neural network that takes in both input streams (even possible different input data types) and outputs a joint prediction. The resulting computation graph of an example of packing 5 different mobile-net like architectures is illustrated in Figure 2. We can do everything to a packed model that we could do to a single neural network. The packed model can be differentiated and the model parameters can be updated. The model can be placed on a device, such as GPU or TPU, as a single unit.

While this gives us scheduling flexibility, there is a major caveat. By packing the models together, we create an artificial synchronization barrier \(^1\). The model can only be differentiated or evaluated as a single unit, and that means that any computation on a packed model has to wait on all of the constituent models. If one of the models is significantly more complex than the others, it will block progress. Likewise, if one of the operations saturates the available compute cores, progress will stall as well. Naive packing leads to a further issue where the input batch has to be synchronized in dimension as well (each model is differentiated or evaluated the same number of times). Therefore, without further thought, the scope of model packing is very narrow.

### 3.1.1 Misaligned Batch Sizes

Requiring that all packed models have the same batch size is highly restrictive, but we can relax this requirement. Our method is to rewrite the packed model to include a dummy operation that pads models with the smaller batch size to match the larger ones in dimension. The pad primitive is exploited for packing models with different batch sizes. The original models are packed and trained based on the batch with the largest size, but the batches for the models with smaller batch sizes will be padded. During training and inference, the padding is sliced and ignored. As depicted in Figure 3, there are a set of original models with batch sizes, the largest training batch size (i.e., 100) is selected and fed to the packed model for a single training step accordingly. Then, the batch with 100 images will be replicated for \(n\) original models in the packed model. The model 1 takes the entire batch, whereas the replicated batches 2, 3, 4, \(n\) are sliced to match the models' requirement (the unused images are discarded after slicing). Thus, all the models can be trained together.

### 3.1.2 Misaligned Step Counts

Another issue with synchronization is that different models may need to be trained for a different number of steps. Even if all of the models are the same, this can happen if the user is trying out different batch sizes. Suppose, we want to train the 2 models for a single epoch consisting of a full size 20,000 images and labels. A batch size of 100 images requires 200 steps and a batch size of 50 requires 400 steps. In such examples, when the earliest model finishes, the packed model has to be check-pointed and reconfigured to only include the remaining models. This introduces a switching overhead of loading and freeing the device memory.

### 3.2 Eliminating Redundancy

Packing forces synchronization which means that dimensional differences between the models or training differences between the models can lead to wasted work. However, packing can allow the system to eliminate redundant computations and data transfers. Consider a hyperparameter tuning use case where we are training the same network with a small architectural tweak:

\[
\text{output1} = \text{nn}_\text{relu} (\text{input1}) \\
\text{output2} = \text{nn}_\text{sigmoid} (\text{input2})
\]

In this case, \text{input1} and \text{input2} refer to the same dataset. We can avoid transferring the batch multiple times by symbolically rewriting the network description to refer to the same input:

[output1 output2] = nn12([input, input])

The potential upside is very significant as it reduces the amount of data transferred along a slower bus like PCI-E. Furthermore, if there are batch size differences, we do not have to pad the models and can simply slice the input data to the appropriate size.

Eliminating redundant computation goes beyond identifying common inputs. Preprocessing is a common practice for machine learning training tasks. There are a number of preprocessing steps might to carry out before training: 1) uniform aspect ratio; 2) image resizing; 3) image normalization;
4) dimension reduction; and 5) data augmentation. Uniform aspect ratio is to ensure that the images have the same size and aspect ratio since most of the deep learning models requires a square shape of input image, thus the cropping is the common operation during this preprocessing. Although we have images with the required aspect ratio, sometimes their size is too large or small, so they have to be scaled to the specified size via resize operation. Image normalization will ensure that each input parameter (e.g., pixel) has a similar data distribution. This normalization usually can be done by subtracting the mean from each pixel and then dividing the result by the standard deviation. Also, in many training jobs images have to be normalized in the range $[0, 1]$ or $[0, 255]$. Dimension reduction usually happens in the case where deep learning performance can be invariant to dimensions, then the RGB channels can be collapsed to a single gray-scale channel. Data augmentation is another common preprocessing method involving augmenting the existing data-set with perturbed versions of the existing images, like rotations and transformations.

When packing models that use the same preprocessing tasks, the pack primitive fuse the steam processing accordingly. In general, packing allows one to eliminate redundant tasks in each models computation graph. Similar ideas can be extended if multiple models have fixed featurization techniques or leverage the same pretrained building blocks.

4 Profiling Model Packing

As it stands, model packing leads to the following tradeoffs. Potential performance improvements include: (1) performing computations (inference and backpropagation) in parallel if and when possible, (2) eliminating redundant data transfers when models are trained on the same dataset, (3) combining redundant computations including preprocessing. On the other hand, the potential overheads include: (1) models that dominate the device resources and block the progress of the others, (2) overhead due to padding misaligned batch sizes, and (3) overhead due to loading and unloading models with a differing number of training steps.

This section describes a series of experiments that illustrate when (what architectures and settings) packing is most beneficial. In particular, we find that packing is most beneficial when the models jointly trained are similar and train on the same dataset.

4.1 Experimental Setup

Our server is 48-core Intel Xeon Silver 4116@2.10GHz with 188GB RAM, running Ubuntu 18.04. The GPU is NVIDIA Quadro P5000. Our evaluation uses 4 models: Multilayer Perceptron with 3 hidden layers (MLP-3), MobileNetV2 [30], ResNet-50 [6], and DenseNet-121 [7] – with all models implemented in TensorFlow 1.14. The default training dataset is 10,000 images from ImageNet [29] and the required input image size of each batch is $224 \times 224$ which is commonly used. Batch sizes start from 32 and goes up to 100 in the experiments [1].

We evaluate packing performance as a function of batch size and the number of models. For each of the models considered in the experiment, we train them simultaneously in a packed configuration. This experiment represents a best case default scenario: the models share the same data and input batch size. Table 1 describes all of the possible configurations involved.

4.2 Metrics

Improvement: We measure the time of single training step of packed model. Since one training epoch can be regarded as a series of repeating training steps and a complete training process is made with multiple epochs, measuring the single training step is sufficient to estimate the performance of the whole training process. We denote the step time as $T_s$ and assume that there are $n$ models (model 1, · · · , $n$), and we compare the time of single training step using packed and sequential approaches.

We first train models 1, · · · , $n$ sequentially (train them one-by-one), and measure the time of single training step which is defined as follows:

$$T_s(Seq) = T_s(Model 1) + \cdots + T_s(Model n)$$

(1)

Then, we packed these models and train the packed model and measure the single training step, which is defined as follows:

$$T_s(Pack) = T_s(Pack(Model 1, \cdots, n))$$

(2)

Thus, we define the improvement metric as follows:

$$IMPV = \frac{T_s(Seq) - T_s(Pack)}{T_s(Seq)}$$

(3)

The improvement metric can quantify the benefits brought by pack primitive, and comparing IMPVs of various training setups can identify performance bottlenecks.

Memory: Fine-grained resource sharing (e.g., training multiple models together on a single device) requires sufficient device memory, thus measuring the memory usage of packed model can provide insights for scheduling different models given a specific device memory capacity. We evaluate the peak of memory usage over the training epoch. This is because if the usage peak is over the GPU memory capacity, the training process will be terminated due to a GPU memory error. We measure the allocated memory and not the active memory used.

Overhead: Training the models in sequence on a single device can bring an additional switching overhead. For example,
the GPU has to unload the old model and the associated context and then load the new models and prepare the context. We train $n$ models in both packed and sequential approaches, but measure the time of the whole training epoch and track the memory usage. We denote $T_e$ as the training time of an epoch, and $T_e(\text{Seq})$ and $T_e(\text{Pack})$ to represent the training time of one epoch for packed and sequential respectively. The switching overhead of training $n$ models is defined as:

$$SwOH = T_e(\text{Seq}) - T_e(\text{Model 1}) - \cdots - T_e(\text{Model n})$$ (4)

However, our hypothesis is that the overhead amortizes over an entire training procedure. This is because $SwOH$ depends on the number of models instead of the number of training steps and epochs. However, a model training usually involves numerous training steps and many training epochs. Thus, compared with a much longer training time, the switch overhead is minor. Nonetheless, our results in section 4.3 illustrate the switching overhead relative to the time of a single optimizer step.

\begin{table}[h]
\begin{tabular}{|l|l|l|}
\hline
Factor & Config & Description \\
\hline
Packing Model & Same & Packing two same models \\
& Different & Packing two different models. To figure out more configuration, we evaluated MLP-3 vs. MobileNet, MobileNet vs. DenseNet-121, ResNet-50 vs. MobileNet, and DenseNet121 vs. ResNet-50. \\
Training Data & Same & All packing models take the same training batch data \\
& Different & All packing models take the different training batch data. \\
Preprocess & Yes & Preprocessing is included in each training step. Training batch are raw image (e.g., JPEG), transferring from disk to GPU. \\
& No & Preprocessing is not included in each training step. Training batch are preprocessed and formatted to binary data before transferring to GPU for each training step. \\
Optimizer & Same & Two models use the same optimizer for single training step, e.g., both of them use Adam optimizer. \\
& Different & Two models use the different optimizer for single training step, e.g., one uses Adam optimizer, the other uses original SGD optimizer \\
Batch Size & Same & Two models take the same batch size for single training step, e.g., both of them take 32 batch size. \\
& Different & Two models take the different batch size for single training step, e.g., one is 32 batch size, the other is 50 batch size. \\
\hline
\end{tabular}
\end{table}

Table 1: Experimental configurations for profiling

4.3 Micro-Benchmarks

Figure 4(a) shows that as the number of packed models increases so do the relative benefits until the resources are saturated. The line of DenseNet-121 ends early because that packing four DenseNet-121 takes too much GPU memory and results in an Out-Of-Memory issue. However, the potential for resources savings is significant. If one is training multiple MLP models, there can be up to a 80% reduction in training time. In short, it is wasteful to allocate entire devices to simple models.

Figure 4(b) illustrates the relationship between batch size and relative improvement when packing two models. The lines of ResNet-50 and DenseNet-121 both end early because the Out-Of-Memory issue emerges when the batch size goes to 80 and 64 respectively. These models are mostly GPU compute bound. Increasing the batch size has a negligible improvement in time even if the packing setup can combine the data transfer. We will see that this story gets more complicated when we consider the effects of preprocessing.

4.4 Ablation Study

To further evaluate the performance of packing models on GPU, we test more cases based on the five factors: (1) whether the packing models have the same architecture, namely packing the same model or not; (2) whether the packing models take the same training data, even multiples of the same model are packed, they still may have to take different training data; (3) whether the packing models take the preprocessed data or raw data to train, i.e., if the preprocessing is included in training; (4) whether the packing models take the same optimizer, and (5) whether packed models have the same training batch size. In this micro-benchmark, we focus on two models to understand the relationship between the training time and the
When we training models with same data since it will reduces the actual training procedure factors. Without loss the generality, we focus on packing two models in this evaluation, packing more models follows the trends as demonstrated in Figure 4. Figure 5 presents the results of micro-benchmark. In the figure, the data points in each sub-figure represent the $T_p(\text{Seq})$ and $T_p(\text{Pack})$ of various configurations with fixing one configuration (e.g., same batch size or same model). The red point (triangle pointed down) indicates that packing two models brings more overhead compared with training them sequentially in this configuration, i.e., $T_p(\text{Pack}) > T_p(\text{Seq})$, while the green point (triangle pointed up) means the opposite. The further from the line, the more significant the performance difference.

As we can see from Figure 5, the best scenarios are where the same training data and same batch size are used. Over all the configurations, the pack primitive always brings benefits when we training models with same data since it will reduces the data transfer. Similar benefits happen with the same batch size configuration. This is important to note because even when the same models are trained but with different data inputs and batch sizes, there can be significant downsides to packing. It is not simply a matter of looking at the neural network architecture, but the actual training procedure factors in to the decision of whether to pack or not.

### 4.5 Memory Usage

We profile the memory usage and the training time of one epoch. Based on the results, we identify the memory usage peak and the switching overhead. We track the GPU memory usage of packing models when the batch size increases, but we particularly care about the memory peak and whether it is beyond the memory capacity and results in an Out-Of-Memory (OOM) error. As depicted in Figure 6, the GPU memory usage peak of MLP-3 model maintains the same as batch size goes up. This is mainly due to two reasons: (1) we find that for simple models TensorFlow’s greedy memory allocation policy over-allocates more GPU’s memory when the actual usage is lower than a specific threshold; (2) the majority of computations for MLP-3 are dot products and are placed on CPU by TensorFlow and do not occupy much GPU memory. Thus, GPU memory usage of single MLP-3 remains the same (the pre-allocation) when the batch size increases.

For convolutional neural networks like ResNet, MobileNet and DenseNet, the GPU memory usage is proportional to the batch size as more intermediate results will be stored as batch size increases. Similarly, when packing two models the GPU memory usage is the sum of memory usage of two models.
4.6 Switching Overheads

We measure the overall training time, and the results are presented in Table 2. As shown in the table, the switching overhead is minor compared to the overall training time and it is even negligible when more epochs are involved in a training process.

| Model          | Seq | Single | Switch OH |
|----------------|-----|--------|-----------|
| MLP-3          | 133 | 61     | 11        |
| MobileNet      | 227 | 107    | 13        |
| ResNet-50      | 274 | 130    | 14        |
| DenseNet-121   | 305 | 144    | 17        |

Table 2: Overall training time (seconds) of 10,000 images and the switch overhead of various models.

4.7 Packing vs CUDA Parallelism

Current NVIDIA GPUs support executing multiple CUDA kernels in parallel. Thus, we conduct an experiment under the same environment as we used on the paper to train models in parallel at the CUDA GPU kernel level. We run multiple simultaneous training processes on TensorFlow. We evaluate this method in the experiments where two processes are boosted at the same time to train the same models (MLP, MobileNet, ResNet, DenseNet) with same optimizer and same batch size (ranging from 32 to 100).

Although CUDA supports it, our results show that it is an inefficient technique. When the models train on the same data, parallel training in isolated kernels leads to duplicated I/O and duplicated data in memory. In the image processing tasks that we consider, the training data batch takes up a substantial amount of memory. We find that in all but the simplest cases lead to an out-of-memory error: "failed to allocate XXX from device: CUDA_ERROR_OUT_OF_MEMORY: out of memory". We also find similar results when the models train on different data—as there is duplicated Tensorflow context information in each of the execution kernels. This error happens all the above experiments except packing the MLP model (due to its lightweight size).

Even with the MLP model, our pack prototype shows benefits at scale. For instance, the training time of single step based on parallel at kernel level is 184ms for both two processes and the packing method takes 200ms. However, as the batch size is increased to 100, the former one takes 1660ms, while the latter one costs 1500ms. We interpret these numbers as an indication that the pack primitive used in this paper is relatively well engineered and incurs small only overheads over the native parallelism in CUDA—overheads that disappear at reasonable batch sizes.

5 Packing-Aware Hyperparameter Search

As we show in the previous section, packing brings the biggest improvement when the models trained are highly similar and train on the same input data. Such a scenario naturally arises in hyperparameter optimization (also called architecture search in this setting). Developers have to search over adjustable parameters such as batch sizes, learning rates, the optimizers, and/or activation functions. Appropriately tuning such hyperparameters is crucial to finding network architectures that generalize to unseen data. In this section, we demonstrate a new hyperparameter tuning algorithm that can take advantage of model packing.

5.1 Hyperband for Hyperparameter Search

We explore how we can extend a state-of-the-art hyperparameter tuning algorithm, Hyperband [19], to better share GPU resources during optimization. Hyperband works by repeatedly sampling random parameter configurations, partially training models with those configurations and discarding those configurations that do not seem promising. Prior work from the community suggests that Hyperband is very effective for parallel hyperparameter search in comparison to sequential algorithms such as Bayesian Optimization [17].

Hyperband poses the search as an online resource allocation problem. Given N discrete neural network configurations to test, it partially trains each configuration and discards those that do not seem promising based on a technique called successive halving. The search routine follows the following structure:

Hyperband(N)

1. for \( r = 1, \ldots, max \)
   a. Randomly sample a set of \( T \) configurations from \( N \) without replacement
   b. for \( i = 1, \ldots, O(\log(r)) \)
      i. Train each of the sample configurations for a number of epochs.
      ii. Calculate the intermediate test error for each sample configuration.
iii. Keep only a fraction of the best configurations for the next iteration.

Intuitively, Hyperband allocates resources to only the most promising configurations. At the maximum iteration, the most promising configurations are trained for the longest. This basic loop can be trivially distributed a random partition $N$ configurations are evaluated on each computational node. Although Hyperband is able to optimize the hyperparameter tuning, the algorithm is long-running since it consists of a large number of trial models/configurations to run and each of them will occupy the entire GPU resource when running.

5.2 Packed Hyperband

Our pack primitive allows Hyperband to jointly train configurations when possible thereby reducing the overall training time. We propose a "packed" Hyperband algorithm that leverages model packing to improve its single-node performance when there are more models to evaluate than available GPU devices. The challenge is to determine which candidate configurations to train jointly and which to train sequentially.

As input, our optimizer will take the random sample $T$ models in each Hyperband step. A packable partitioning is a grouping of $T$ models such that each group can fit on a single device, i.e., packing configurations that do not exceed the amount of memory of the GPU. The optimization problem is to search over all packable partitions to find the best possible configuration (one that maximizes the overall run time). Note that the singleton partitioning (every single model) is always a viable solution and potentially even an optimal solution. We call this primitive pack_opt($T$), which solves the search problem to produce feasible packing configuration. Accordingly, we can run a modified Hyperband loop that packs models when beneficial:

\[
Packed_{Hyperband}(N)
\]

1. for $r = 1, ..., max$
   (a) Randomly sample a set of $T$ configurations from $N$ without replacement
   (b) pack_opt($T$)
   (c) for $i = 1, ..., O(\log(t))$
      i. Train each of the sample configurations for a number of epochs.
      ii. Calculate the intermediate test error for each sample configuration.
      iii. Keep only a fraction of the best configurations for the next iteration.

5.3 Heuristic Solution

There are two challenges to solving this problem: (1) developing an accurate cost model to evaluate the cost of a packed plan, and (2) a search algorithm that can effectively scale with $T$. Of course, the combinatorial nature of this problem makes both (1) and (2) hard to accomplish optimally and we need a heuristic to address this problem. Recognizing that models that are similar pack well together, we design a nearest-neighbor based heuristic.

The method randomly selects a single configuration (out of $T$) as the centroid and packs all other configurations similar to it until the device runs out of memory. This process is repeated until all models are packed or determined that the best choice is to run them sequentially. For calculating the similarity, we map hyperparameter configurations to multidimensional feature space and measure the pairwise Euclid distance among all the configurations. A user turned similarity threshold trades off how aggressively the system will pack models. For example, considering the sampled hyperparameter configurations is shown in the Table 3, we take standard distance unit as 1, and compute the distance between any two configurations. For categorical hyperparameters like optimizer and activation, the distance is 0 if same and 1 if different, for numeric hyperparameters, we use the index to compute distance. So, the distance between configuration $A$ [batch size:20, optimizer: SGD, learning rate:0.01, activation: ReLu] and configuration $B$ [batch size:40, optimizer: Adagrad, learning rate:0.01, activation: ReLu] is 5.

5.4 Evaluation

The goals of out evaluation are two fold: first to demonstrate that packing can significantly improve hyperparameter search performance and second to evaluate our packing optimizer. We conduct the experiments based on the same hardware environment as illustrated in section 4.1. We examine the Hyperband variants on CIFAR-10 [14] which consists of 60000 color $32 \times 32$ images in 10 classes (50000 for training dataset, 10000 for testing dataset). The system’s goal is to find the best configuration of those described in Table 3, thus all hyperparameter configuration is the combination of all hyperparameters which has 1056 configurations in total. The input of Hyperband, $R$ and $\eta$, are set to 81 and 3, according to the original Hyperband paper [19].

| Hyperparameter | Value |
|----------------|-------|
| Batch size     | 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70 |
| Optimizer      | Adam, SGD, Adagrad, Momentum |
| Learning Rate  | 0.000001, 0.00001, 0.0001, 0.001, 0.01, 0.1 |
| Activation     | Sigmoid, Leaky ReLu, Tanh, ReLu |

Table 3: Hyperparameter configurations for evaluation

We compare our pack optimizer against two other heuristic strategies:

Random Pack Hyperband: After sampling hyperparameter configurations, the method randomly selects $m$ configurations
to pack and evaluate them together, then keep the best $n$ configurations and discard the rest as the original Hyperband does.

**Batch-size Pack Hyperband**: Rather than randomly selecting, Batch-size Pack Hyperband only pack the models with the same batch size. Although the number of packed models are confined by GPU memory size, and greedy method is employed to resolve the issue, i.e. packing as many models as possible until fully usage.

We evaluate the overall running time of Hyperband with the different pack_opt algorithms. As presented in the Table 4, all the pack-based Hyperband variants can reduce the running time w.r.t the original Hyperband algorithm for all scenarios. Our proposal, kNN Pack Hyperband, achieves the best performance since it takes advantages of our findings from the previous section where packing the most similar models leads to the biggest improvements. The conclusion is that such an approach can save time (and consequently money) in real end-to-end tasks. A simpler heuristic, Batch-size Pack Hyperband, is not as effective because it under-utilizes the available GPU resources by missing packing opportunities with models with slightly different batch sizes. We include this baseline because some prior work has proposed packing-like primitives that only support equal batch sizes [26]. To emphasize this point, a Random Pack Hyperband can save more time than Batch-size Pack Hyperband since it achieves a better GPU resource utilization. Our kNN strategy gets the best of both worlds: it finds the most beneficial packing opportunities while completely utilizing the available resources, and benefits are scalable when deployed in an environment with larger GPU resource.

| Dataset      | Original | Batch-size | Random | kNN     | Speedup |
|--------------|----------|------------|--------|---------|---------|
| MLP-3        | 9236s    | 5260s      | 3682s  | 3491s   | up to 2.7× |
| MobileNet    | 52092s   | 45787s     | 36973s | 30182s  | up to 1.7× |
| ResNet-50    | 98067s   | 89162s     | 75436s | 70047s  | up to 1.4× |
| DenseNet-121 | 131494s  | 126437s    | 117405s| 108673s | up to 1.2× |

Table 4: Performance of pack-based Hyperband

## 6 Related Work

Given the high cost of GPU resources and the prevalence of machine learning, building multi-tenant system for machine learning deployment is becoming increasingly important. There are number of systems that attempt to control resource usage in machine learning, specifically memory optimization [10, 15, 32, 37, 40], but we see this problem as complementary. We focus on related work that studies placement in machine learning and hyperparameter tuning systems.

### 6.1 Systems for Hyperparameter Tuning

Since hyperparameter tuning and neural network architecture search are crucial parts of the machine learning development process, a number of systems have been proposed to scale up such search routines. For example, Google Vizier [3] exposes hyperparameter search as a service to its organization’s data scientists. Aggressive "scale-out" has been the main design principle of Vizier and similar systems [16, 19, 22].

Recently, there has been a trend towards a more controlled resource usage. CHOPT [11] proposes a novel stop-and-go scheme that can take advantage of transient cloud based resources. HyperSched [21], proposes a scheduling framework for hyperparameter tuning tasks when there are contended specialized resources. And, some work has been done on resource management [33] and pipeline re-use [18] in the non-deep learning setting. We believe that pack and pack_opt are two core primitives that are useful in neural network hyperparameter tuning when specialized hardware such as GPUs and TPUs are used.

### 6.2 Coarse-grained Multi-tenancy

Most current projects about building multi-tenant system for machine learning deployment is based on device-level placement, i.e., dividing resources at the granularity of full devices (e.g., an entire server or GPU), which we refer to as coarse-grained multi-tenancy. Here, the scheduler partitions a cluster of servers where each server has one or more GPUs for various model training tasks and seeks to reduce the overall training time by intelligent placement. One of the earliest works in this space was the TetriSched project, which considered how to specify and optimize locality constraints during process scheduling [35]. Project Philly analyzed a trace of machine learning workloads run on a large cluster of GPUs in Microsoft and indicated the trade-off between locality and GPU utilization [9]. Other scheduling methods have followed, such as Tiresias [4] and Optimus [28]. Several extensions have been proposed to this basic line of work including fairness [24], pre-emption [39], performance prediction [41], and network traffic scheduling [8, 23]. According to the recent study [5], co-locating data and computation and exploiting the characteristics of different workloads are two factors that can affect the performance when training machine learning models in a data center.

### 6.3 Fine-grained Multi-tenancy

There are a number of projects which attempt to achieve the fine granularity. This idea called packing, which has been discussed in three prior works [13, 26, 38]. Gandiva is a cluster scheduling framework for deep learning jobs that provides primitives such as time-slicing and migration to schedule different jobs, it supports packing as well, implementing packing arrangements using a greedy algorithm without decent
optimizations. Narayanan et al. [26] discuss a packing idea that tries to combine various models and trains them together. However, this proposed packing method of layer fusion has limited application scenarios as it only focuses on models with the same batch size, whereas our work is more general and support different batch size, which bring more optimization opportunities for the future work. We particularly note that in Narayanan et al.: (1) the largest evaluated network was AlexNet from 2012, (2) there is no discussion about training batch size, (3) there is no ablation study that differentiates performance wins from variable elimination v.s. improved parallelism and utilization, and (4) the paper does not mention the potential for packed models to train slower than the sum of their parts, which is only apparent with modern architectures. We take these limitations as inspiration for our work and present a packing framework that is performant enough to run on state-of-the-art computer vision models and train with modern architectures and modern training configurations.

Our approach is similar to Krishnan et al.’s high-level proposal [13], but we study if and when packing is beneficial. Therefore, compared with these previous works, our prototype implements a general packing method that can pack various models with different batch sizes. Since we believe that fine-grained optimization and scheduling will be a core component of any future large-scale deep learning system, this paper offers an elaborate performance study of packing method.

6.4 Multi-tenancy Systems

CROSSBOW is a system for training deep learning models that enables users to select a small batch and scale to multiple GPUs [12], i.e., multi-tenancy for scaling the selected small batch size. PipeDream is a deep neural network training system for GPUs that parallelizes computation by pipelining execution across multiple machines that partitions and pipelines training jobs across worker machines [25]. Some related projects consider shared multi-user machine learning services. Ease.ml is a declarative machine learning service platform [20]. It mainly focuses on a cost-aware model selection problem in a multi-tenant system. Here, the users have no idea which model can achieve the promising results, and therefore ease.ml has to generate a sequence of models to train to maximize accuracy. Although these works concentrate on taking advantage of multi-tenancy for deep learning instead of designing multi-tenancy systems, our performance evaluation can serve as guidelines that could help future research and development of multi-tenancy-support systems.

7 Discussion and Limitations

Our core contribution is evaluating an optimized model packing framework on state-of-the-art neural network models. Our evaluation uncovered performance bottlenecks not discussed in prior work, such as the potential for packed models to train slower than the sum of their parts, which we feel is a valuable experimental contribution to the community. However, it is worth noting that prior work in model packing is very nascent (over the last year), and our paper does contribute a technique for training packed models with different training batch sizes that prior work ignores. With this additional complexity, there is a need to optimize packed configurations and we further contribute a nearest-neighbor heuristic to do so.

While, we focus our experiments on hyperparameter tuning. We believe that the pack primitive and the optimization of packing configurations is generally useful and will be a core part of any multitienancy framework for deep learning. In hyperparameter tuning there is a single-user and a clear SLO (find the best model over all). To extend to more general settings where concurrent models are trained, we will have to reason about multiple users, priorities, and user-specified objectives.

Although our long-term goal is to build a system for multi-tenant deep learning deployment, we decide to make a deep investigation on single GPU so that we will know how to optimize when there are multiple GPUs. Therefore, any distributed training and the regarding optimization is out of the scope of the paper. We take advantage of TensorFlow API to build the prototype system. Although we believe that a custom execution platform could improve performance, however for this step we focus packing as a higher-level primitive due to (1) the optimizations will be more transferable across ML execution frameworks and thus increase the impact or applicability of our insights, and (2) many low-level libraries are highly optimized and introducing these changes (e.g. supporting jagged arrays) we believe are interesting research questions on their own.

8 Conclusion and Future Work

We analyze the benefits and limitations of packing multiple models together to take advantage of available GPU resources for model training. Under the proper conditions, this packing can bring up to 40% reduction in latency per model packed, compared with training the models sequentially on a GPU. We develop an optimize to heuristically select the most beneficial packing configurations. We demonstrate that this primitive can be used to accelerate a state-of-the-art hyperparameter tuning algorithm. Our end-to-end tuning system demonstrates a 2.7x speedup in terms of time to find the best model by improving GPU utilization. Our analysis opens many interesting optimization opportunities, such as the training process can be decomposed and scheduled for packing to reduce the overall training time, or trading off accuracy or training time to improve overall resource utilization.
References

[1] Yoshua Bengio. Practical recommendations for gradient-based training of deep architectures. In Neural Networks: Tricks of the Trade - Second Edition, pages 437–478. Springer, 2012.

[2] Alfredo Canziani, Adam Paszke, and Eugenio Culurciello. An analysis of deep neural network models for practical applications. arXiv preprint arXiv:1605.07678, 2016.

[3] Daniel Golovin, Benjamin Solnik, Subhodeep Moitra, Greg Kochanski, John Karro, and D Sculley. Google vizier: A service for black-box optimization. In Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 1487–1495. ACM, 2017.

[4] Juncheng Gu, Mosharaf Chowdhury, Kang G. Shin, Yibo Zhu, Myeongjae Jeon, Junjie Qian, Hongqiang Harry Liu, and Chuanxiong Guo. Tiresias: A GPU cluster manager for distributed deep learning. In USENIX Symposium on Networked Systems Design and Implementation (NSDI), pages 485–500, 2019.

[5] Kim M. Hazelwood, Sarah Bird, David M. Brooks, Soumith Chintala, Utku Diril, Dmytro Dzhulgakov, Mohamed Fawzy, Bill Jia, Yangqing Jia, Aditya Kalro, James Law, Kevin Lee, Jason Lu, Pieter Noordhuis, Misha Smelyanskiy, Liang Xiong, and Xiaodong Wang. Applied machine learning at facebook: A datacenter infrastructure perspective. In IEEE International Symposium on High Performance Computer Architecture (HPCA), pages 620–629, 2018.

[6] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Identity mappings in deep residual networks. In European Conference on Computer Vision (ECCV), pages 630–645, 2016.

[7] Gao Huang, Zhuang Liu, Laurens van der Maaten, and Kilian Q. Weinberger. Densely connected convolutional networks. In IEEE Conference on Computer Vision and Pattern Recognition (CVPR), pages 2261–2269, 2017.

[8] Xin Sunny Huang, Ang Chen, and T. S. Eugene Ng. Green, yellow, yield: End-host traffic scheduling for distributed deep learning with tensorlights. In IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), pages 430–437, 2019.

[9] Myeongjae Jeon, Shivaram Venkataraman, Amar Phanishayee, Junjie Qian, Wencong Xiao, and Fan Yang. Analysis of large-scale multi-tenant GPU clusters for DNN training workloads. In USENIX Annual Technical Conference (ATC), pages 947–960, 2019.

[10] Hai Jin, Bo Liu, Wenbin Jiang, Yang Ma, Xuanhua Shi, Bingsheng He, and Shaofeng Zhao. Layer-centric memory reuse and data migration for extreme-scale deep learning on many-core architectures. ACM Transactions on Architecture and Code Optimization (TACO), 15(3):37, 2018.

[11] Jinwoong Kim, Minkyu Kim, Heungseok Park, Ernar Kusdavletov, Dongjun Lee, Adrian Kim, Ji-Hoon Kim, Jung-Woo Ha, and Nako Sung. Chopt: Automated hyperparameter optimization framework for cloud-based machine learning platforms. arXiv preprint arXiv:1810.03527, 2018.

[12] Alexandros Koliousis, Pijika Watcharapichat, Matthias Weidlich, Luo Mai, Paolo Costa, and Peter R. Pietzuch. Crossbow: Scaling deep learning with small batch sizes on multi-gpu servers. PVLDB, 12(11):1399–1413, 2019.

[13] Sanjay Krishnan, Aaron J Elmore, Michael Franklin, John Paparrizos, Zechao Shang, Adam Dziedzic, and Rui Liu. Artificial intelligence in resource-constrained and shared environments. ACM SIGOPS Operating Systems Review, 53(1):1–6, 2019.

[14] Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. Technical report, Citeseer, 2009.

[15] Tung D Le, Haruki Imai, Yasushi Negishi, and Kiyokuni Kawachiya. Tlms: Large model support in tensorflow by graph rewriting. arXiv preprint arXiv:1807.02037, 2018.

[16] Liam Li, Kevin Jamieson, Afshin Rostamizadeh, Ekaterina Gonina, Moritz Hardt, Benjamin Recht, and Ameet Talwalkar. Massively parallel hyperparameter tuning. arXiv preprint arXiv:1810.05934, 2018.

[17] Liam Li, Kevin G. Jamieson, Afshin Rostamizadeh, Ekaterina Gonina, Moritz Hardt, Benjamin Recht, and Ameet Talwalkar. Massively parallel hyperparameter tuning. CoRR, abs/1810.05934, 2018.

[18] Liam Li, Evan Sparks, Kevin Jamieson, and Ameet Talwalkar. Exploiting reuse in pipeline-aware hyperparameter tuning. arXiv preprint arXiv:1903.05176, 2019.

[19] Lisha Li, Kevin G. Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, and Ameet Talwalkar. Hyperband: A novel bandit-based approach to hyperparameter optimization. J. Mach. Learn. Res., 18:185:1–185:52, 2017.

[20] Tian Li, Jie Zhong, Ji Liu, Wentao Wu, and Ce Zhang. Ease,ml: Towards multi-tenant resource sharing for machine learning workloads. PVLDB, 11(5):607–620, 2018.
[21] Richard Liaw, Romil Bhardwaj, Lisa Dunlap, Yitian Zou, Joseph E Gonzalez, Ion Stoica, and Alexey Tumanov. Hypersched: Dynamic resource reallocation for model development on a deadline. In Proceedings of the ACM Symposium on Cloud Computing, pages 61–73, 2019.

[22] Richard Liaw, Eric Liang, Robert Nishihara, Philipp Moritz, Joseph E Gonzalez, and Ion Stoica. Tune: A research platform for distributed model selection and training. arXiv preprint arXiv:1807.07118, 2018.

[23] Hyeontaek Lim, David G Andersen, and Michael Kaminsky. 3lc: Lightweight and effective traffic compression for distributed machine learning. arXiv preprint arXiv:1802.07389, 2018.

[24] Kshiteej Mahajan, Arjun Singhvi, Arjun Balasubramanian, Varun Batra, Surya Teja Chavali, Shivaram Venkataraman, Aditya Akella, Amar Phanishayee, and Shuchi Chawla. Themis: Fair and efficient gpu cluster scheduling for machine learning workloads. arXiv preprint arXiv:1907.01484, 2019.

[25] Deepak Narayanan, Aaron Harlap, Amar Phanishayee, Vivek Seshadri, Nikhil Devanur, Greg Granger, Phil Gibbons, and Matei Zaharia. Pipedream: Generalized pipeline parallelism for dnn training. In ACM Symposium on Operating Systems Principles (SOSP), 2019.

[26] Deepak Narayanan, Keshav Santhanam, Amar Phanishayee, and Matei Zaharia. Accelerating deep learning workloads through efficient multi-model execution. In NIPS Workshop on Systems for Machine Learning, 2018.

[27] NVIDIA. Nvidia virtual gpu technology. https://www.nvidia.com/en-us/design-visualization/technologies/virtual-gpu/, 2019.

[28] Yanghua Peng, Yixin Bao, Yangrui Chen, Chuan Wu, and Chuanxiong Guo. Optimus: an efficient dynamic resource scheduler for deep learning clusters. In European Conference on Computer Systems (EuroSys), pages 3:1–3:14, 2018.

[29] Olga Russakovsky, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael Bernstein, Alexander C. Berg, and Li Fei-Fei. ImageNet Large Scale Visual Recognition Challenge. International Journal of Computer Vision (IJCV), 115(3):211–252, 2015.

[30] Mark Sandler, Andrew G. Howard, Menglong Zhu, Andrey Zhmoginov, and Liang-Chieh Chen. Mobilenetv2: Inverted residuals and linear bottlenecks. In IEEE Conference on Computer Vision and Pattern Recognition (CVPR), pages 4510–4520, 2018.

[31] Roy Schwartz, Jesse Dodge, Noah A Smith, and Oren Etzioni. Green AI. arXiv preprint arXiv:1907.10597, 2019.

[32] Taro Sekiyama, Takashi Imamiichi, Haruki Imai, and Rudy Raymond. Profile-guided memory optimization for deep neural networks. arXiv preprint arXiv:1804.10001, 2018.

[33] Evan R Sparks, Ameet Talwalkar, Daniel Haas, Michael J Franklin, Michael I Jordan, and Tim Kraska. Automating model search for large scale machine learning. In Proceedings of the Sixth ACM Symposium on Cloud Computing, pages 368–380. ACM, 2015.

[34] Emma Strubell, Ananya Ganesh, and Andrew McCallum. Energy and policy considerations for deep learning in NLP. In Annual Meeting of the Association for Computational Linguistics (ACL), pages 3645–3650, 2019.

[35] Alexey Tumanov, Timothy Zhu, Jun Woo Park, Michael A Kozuch, Mor Harchol-Balter, and Gregory R Ganger. Tetrisched: global rescheduling with adaptive plan-ahead in dynamic heterogeneous clusters. In European Conference on Computer Systems (EuroSys), page 35, 2016.

[36] Carl A Waldspurger. Memory resource management in vmware esx server. ACM SIGOPS Operating Systems Review, 36(SI):181–194, 2002.

[37] Linnan Wang, Jinmian Ye, Yiyang Zhao, Wei Wu, Ang Li, Shuaiwen Leon Song, Zenglin Xu, and Tim Kraska. Superneurons: dynamic GPU memory management for training deep neural networks. In ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP), pages 41–53, 2018.

[38] Wencong Xiao, Romil Bhardwaj, Ramachandran Ramjee, Muthian Sivathanu, Nipun Kwatra, Zhenhua Han, Pratyush Patel, Xuan Peng, Hanyu Zhao, Quanlu Zhang, et al. Gandiva: Introspective cluster scheduling for deep learning. In USENIX Symposium on Operating Systems Design and Implementation (OSDI), pages 595–610, 2018.

[39] Hidehito Yabuuchi, Daisuke Taniwaki, and Shingo Omura. Low-latency job scheduling with preemption for the development of deep learning. In USENIX Conference on Operational Machine Learning (OpML), pages 27–30, 2019.

[40] Junzhe Zhang, Sai Ho Yeung, Yao Shu, Bingsheng He, and Wei Wang. Efficient memory management for gpu-based deep learning systems. arXiv preprint arXiv:1903.06631, 2019.
[41] Haoyue Zheng, Fei Xu, Li Chen, Zhi Zhou, and Fangming Liu. Cynthia: Cost-efficient cloud resource provisioning for predictable distributed deep neural network training. In International Conference on Parallel Processing (ICPP), pages 86:1–86:11, 2019.