Orchestrate: Infrastructure for Enabling Parallelism during Hyperparameter Optimization

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Abstract

Two key factors dominate the development of effective production grade machine learning models. First, it requires a local software implementation and iteration process. Second, it requires distributed infrastructure to efficiently conduct training and hyperparameter optimization. While modern machine learning frameworks are very effective at the former, practitioners are often left building ad hoc frameworks for the latter. We present SigOpt Orchestrate, a library for such simultaneous training in a cloud environment. We describe the motivating factors and resulting design of this library, feedback from initial testing, and future goals.

1 Introduction

Deep learning models have enjoyed broad adoption [8] because of the development of popular libraries, such as MXNet [5], PyTorch [10] and Tensorflow [1]. These libraries have provided an efficient and stable framework in which to develop models.

For these deep learning models to perform well, meta-decisions regarding their architecture and hyperparameters must be made; conducting this model tuning efficiently presents a challenge both in terms of strategy and implementation. Often times, the strategy for hyperparameter tuning involves defining some measurement of generalization quality for a given model and then using a black-box optimization strategy to find an optimal configuration [7]. Suitable strategies include grid search [3], random search [2], evolutionary strategies [14], swarm intelligence methods [4], and Bayesian optimization [6, 11].

Each of these strategies requires training a model many times, each with different hyperparameters/architecture. Training several models in parallel can reduce the necessary wall clock time required to complete this important step. Running multiple models in a local development environment is likely infeasible, usually because of the specialized hardware required for deep learning models. As such, distributed infrastructure for parallel model trainings is a necessary component of an efficient model building pipeline. Deep learning models also require a great deal of high quality labeled data, but this topic is not discussed in this article.

We present a library, Orchestrate, which seeks to manage the infrastructure complications fundamental to parallel hyperparameter tuning. Orchestrate was designed to work with SigOpt, a cloud-based optimization API for hyperparameter tuning in parallel [9]. The goal of Orchestrate is to provide the necessary infrastructure to coordinate and simultaneously execute multiple hyperparameter configurations suggested by SigOpt; this allows the user to focus on the actual design of the deep learning model rather than the infrastructure used during hyperparameter tuning.

In this paper, we discuss the circumstances which led us to develop Orchestrate and the design decisions made to address these circumstances. We present an internal use case (conducted during alpha testing) and goals for future development.

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2 Initial investigation and understanding expectations

Many organizations face the need to develop scalable infrastructure to support tools that have been developed in a local environment. Airflow\(^1\) was developed at AirBnB to implement and monitor sequences of tasks in a distributed and asynchronous environment. Mesosphere\(^2\) provides enterprise solutions around deploying containers to public clouds. Uber has developed Michelangelo\(^3\) to provide internal teams the ability to deploy their machine learning tools at scale.

To inform the development of Orchestrate, we interviewed SigOpt users (and, particularly, deep learning users who evaluate multiple models in parallel) to understand what was needed for Orchestrate to be effective. Below, we summarize the responses and the resulting Orchestrate workflow.

2.1 Parallelism

At the highest level, interviewees stated that they want the power to execute multiple hyperparameter optimization experiments simultaneously (to accelerate the optimization process); furthermore, each of these experiments could have drastically different compute times. Within a single experiment, interviewees wanted to be able to leverage evaluating multiple model configurations simultaneously. Even within a single model configuration evaluation, interviewees wanted to distribute their model across multiple GPUs and evaluate multiple cross-validation folds simultaneously. When initially scoping Orchestrate, we had anticipated the desire to support evaluating multiple models in parallel, but, after the interviews, it became clear that for this project to be successful we would have to address parallelism on multiple levels.

2.2 On Demand Cluster

Experimental model development may proceed at an erratic pace; interviewees reported needing significant compute resources at inconsistent intervals because of the development / tuning cycle at their company. Additionally, these interviewees were hoping to leverage the elastic nature of cloud computing to have access to the resources they needed, when they needed them.

2.3 Heterogeneous Resources

In combining the desire to limit compute cost with a desire to tune multiple models simultaneously (mentioned in Section 2.1), we realized that the cluster should be able to support heterogeneous compute resources. Both CPU and GPU machines should be available within the same cluster to allow models which do not require GPU resources to not have to pay for them.

2.4 Monitoring

In entrusting Orchestrate to manage the infrastructure, interviewees voiced concern about loss of proximity to the actual functioning of the model tuning experiment; in our interviews we learned that they still want to be able to monitor the process despite abstracting away some of the details.

Monitor status The process of monitoring Orchestrate status seemed to split into two key factors: the status of the cluster and the status of individual experiments on the cluster. Effective monitoring of Orchestrate would require both the ability to answer the question “Is the cluster infrastructure operating as planned?” and the question “How is work being distributed for each of my experiments?”

View Logs A common fear among interviewees was that if the infrastructure were managed by Orchestrate that they would lose the ability to easily detect and rectify mistakes in their models. This is especially complicated in situations where their models could behave very differently for different model configurations. The proposed solution was to be able to easily access logs from experiments as they were running (or after they crashed). In particular, interviewees wanted to be able to easily recover all the logs associated with a single experiment, irrespective of what other experiments were running on the cluster or how parallel model configurations were distributed.

\(^1\)https://airflow.apache.org/
\(^2\)https://mesosphere.com
\(^3\)https://eng.uber.com/michelangelo/
Monitor performance Perhaps most importantly, interviewees wanted to be able to monitor the actual quality of the models as they went through this model tuning process. Because this was already managed through the SigOpt website, it was not considered as a component of Orchestrate.

2.5 Stopping Experiments

Interviewees stated that hyperparameter optimization can surface bugs within their models, whether due to their code throwing exceptions or their model’s performance failing to reach a threshold. In both circumstances, interviewees wanted the ability to terminate all execution on their experiment and free up the resources for future work.

2.6 Resulting workflow from our investigation

The Orchestrate workflow, as guided by these customer discussions, is depicted in Figure 1. Of particular note is that the creation and destruction of the cluster is dissociated from the running of experiments. This allows multiple experiments to be run on a single cluster (rather than tying the existence of a cluster to a single experiment) and it allows model tuning artifacts (such as model-generated logging output) to remain available after the experiment has completed.

![Figure 1: The results of our investigation into a workflow to support prospective users of Orchestrate with the parallel components of their hyperparameter optimization.](image)

3 Design and Implementation

3.1 Command Line Interface

Because our customers have a variety of modeling backgrounds and goals, we prioritized building a model agnostic tool. This tool could be installed anywhere on a user’s system, and could be used to containerize models that lived anywhere. We also wanted our tool to be language-agnostic, so that even if our tool is written in Python, it can be used from any environment, on any kind of model.

Our core API commands are listed below; they, respectively, allow a user to create a cluster, start an experiment, monitor experiment status, view experiment logs, delete an experiment, and destroy an experiment.

```
sigopt cluster create -f cluster_configuration.yml
sigopt run -f experiment_configuration.yml
sigopt status $EXPERIMENT_ID
sigopt logs --follow $EXPERIMENT_ID
sigopt delete $EXPERIMENT_ID
sigopt cluster destroy -n $CLUSTER_NAME
```
3.2 Containerization

To fulfill our goal of allowing customers to take their locally developed models and tune them in the cloud, we needed a mechanism for moving a model (and all its supporting components). We found containers to be a logical solution for managing the process. This process is less brittle than copying individual files and more flexible than attempting to provide customers with pre-defined hard disc images already loaded with standard dependencies. Orchestrate uses Docker, an industry standard tool for containerization.

One remaining point of contention when using containers is how to move/access data from which a model should be trained; at present, we advise users import their data from a cloud source after the container has started. Devising a strategy for reducing data traffic is a priority going forward.

3.3 Kubernetes

If containers are the emerging standard for wrapping up code and dependencies, Kubernetes is the emerging standard for running containers. It is not purpose-built for machine learning (the stated goal of many of our users), but it has many features desired of Orchestrate clusters, such as facilitating communication between machines, starting containers across multiple machines, and managing running containers. Kubernetes provides built-in APIs and abstractions for starting jobs, monitoring infrastructure, and viewing container logs, and other important functions. During our development of Orchestrate we relied heavily on the standard Kubernetes paradigms (such as jobs, pods and containers) and APIs. Using these built-in tools shaved weeks off of our development cycle.

Additionally, managed Kubernetes implementations are hosted by Amazon, Google and Azure clouds. This allowed us to save development time by relying on a managed Kubernetes implementation without being locked-in to one cloud provider.

3.4 AWS and EKS

We chose Amazon Web Services (AWS) as our cloud provider because it was an environment that our early interviewees were familiar with and comfortable using. AWS released their Elastic Kubernetes Service (EKS) shortly after we began scoping this project. To facilitate transfer of containers from local environments to an EKS cluster, we use AWS Elastic Container Registry (ECR). Furthermore, EKS allows users to create clusters with both CPU and GPU machines within the same cluster; this helps support the “multiple experiments, one cluster” goal described in Section 2.2.

EKS came with a few limitations, however. EKS is billed separately from AWS machines, so while the cost of one EKS cluster may be negligible compared to a GPU machine, it is still an additional cost. Additionally, as of this article, AWS limits each account to three EKS instances by default. To avoid friction from requiring customers contact AWS support to exceed that limit, we opted to build a workflow for a team to share a single cluster to run multiple experiments.

We expect to integration Orchestrate with every other cloud over time so it is fully agnostic to the underlying infrastructure as we progress toward GA.

3.4.1 Cluster Configuration

AWS EKS simplifies the process of creating a Kubernetes cluster on AWS, but it still requires knowledge of the AWS and Kubernetes APIs. With Orchestrate, we wanted to go one step further in reducing the complication of spinning up a cluster. When the user creates a cluster, they provide us with a short model configuration yaml file listing the cluster name, cloud provider (only AWS for now), and desired number and type of GPU and / or CPU

```yaml
# Cluster Config file: demo.yml
cloud_provider: aws
cluster_name: orchestrate-cluster
gpu:
  instance_type: p3.8xlarge
  min_nodes: 4
  max_nodes: 4
cpu:
  instance_type: c4.xlarge
  min_nodes: 4
  max_nodes: 4
```

Figure 2: Example cluster configuration yaml file
resources. From this, Orchestrate manages spinning up and connecting the necessary cloud resources behind the scenes.

3.5 Experiments

Orchestrate relies heavily on SigOpt’s centralized API for distributed hyperparameter optimization to run model tuning experiments with simultaneous model evaluations. SigOpt also informs Orchestrate on the progress of the experiment so that experiments can be run for the desired duration (this information can also be recovered from the CLI to monitor experiment status). Additionally, use of the SigOpt API for experiments allows us to take advantage of the SigOpt web interface to view and share experiments, as shown in Figure 3.

SigOpt serves as a system of record for completed experiments. While some experiment artifacts, such as container logs, will be lost once the cluster is destroyed, experiment metadata, including parameters and performance will exist on SigOpt in perpetuity.

![Orchestrate SGD Classifier (python)](https://sigopt.com)

**Figure 3:** An in-progress Orchestrate experiment, viewed on [https://sigopt.com](https://sigopt.com)

3.5.1 Experiment Configuration

For experiments requiring GPUs, users may provide the number of GPUs needed per model in their experiment configuration yaml file. Orchestrate passes this information to Kubernetes for use in creating a job on the cluster, and the Kubernetes scheduler manages resource and capacity limitations in the cluster. The experiment configuration yaml file is where the user defines the experiment structure (number of different configurations with which they wish to evaluate their model and how many of those evaluations may be run in parallel).

3.6 Limitations

**Models in Development**  Because of our focus on model evaluations in parallel, we have not built features and visualizations, etc., that could be useful for a practitioner during early development.

**User-provided containers**  Because Orchestrate packages a model, dependencies, and Orchestrate-specific code into a Docker container, allowing a user to bring their own model container would run into a technical constraint of running Docker within Docker.

**Non-Kubernetes Cluster Management**  At present, this tool does not play nicely with in house clusters that are not Kubernetes based. Specifically, we cannot support clusters running Slurm, a popular workload manager for universities.
High-GPU Models  The largest GPU instance type provided by AWS currently has 8 GPUs (p3.16xlarge); because Orchestrate currently only supports using AWS, and we have not tested a model exceeding the constraints of one AWS EC2 instance, a single model configuration cannot be trained on more than 8 GPUs simultaneously.

Figure 4: A split-screen terminal showing two SigOpt Orchestrate CLI commands. On the top is “sigopt status $ EXPERIMENT_ID”, and on the bottom is “sigopt logs -follow $ EXPERIMENT_ID”. The green and blue colors in the logs represent output from two distinct simultaneous evaluations of the model.

4 Initial Feedback

Our initial alpha tester used Orchestrate over the course of several weeks during his development of a convolutional neural network with 3 convolutional layers and 2 fully connected layers. This neural network was trained on the German traffic sign dataset [12], and each model required training on one GPU. During each model tuning experiment with Orchestrate the model was evaluated 300 times, with fifteen models evaluated simultaneously.

The alpha tester said that, in addition to being happy with the numerical results of the hyperparameter optimization, Orchestrate was “easy to use—I was able to get up and running very fast.” The constructive feedback aligned with some of our earlier thoughts on Orchestrate’s limitations. Specifically, the alpha tester found that Orchestrate was “a useful tool once you’ve defined your model but hard if you want to make incremental changes.” The user also stated that he found the ability to extract logs during and after the run to be “helpful”.

5 Future Work

High priority areas for future work include:

- Incorporating information about how much storage or computational resources each model requires.
- Efficient dataset storage on the cluster. Good strategies for managing this have been discussed at the NIPS ML Systems workshop [13].
- Connecting to existing Kubernetes clusters not created by Orchestrate.
- Supporting other cloud providers.
• Meet new collaborators to understand the needs of specific use cases, e.g., reinforcement learning or natural language processing.

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