CrossedWires: A Dataset of Syntactically Equivalent but Semantically Disparate Deep Learning Models

Max Zvyagin, Thomas Brettin, Arvind Ramanathan
Argonne National Laboratory
Lemont IL 64309
{mzvyagin,brettin,ramanathana}@anl.gov

Sumit K. Jha
Computer Science Department
University of Texas at San Antonio
sumit.jha@utsa.edu

Abstract

The training of neural networks using different deep learning frameworks may lead to drastically differing accuracy levels despite the use of the same neural network architecture and identical training hyperparameters such as learning rate and choice of optimization algorithms. Currently, our ability to build standardized deep learning models is limited by the availability of a suite of neural network and corresponding training hyperparameter benchmarks that expose differences between existing deep learning frameworks. In this paper, we present a living dataset of models and hyperparameters, called CrossedWires, that exposes semantic differences between two popular deep learning frameworks: PyTorch and Tensorflow. The CrossedWires dataset currently consists of models trained on CIFAR10 images using three different computer vision architectures: VGG16, ResNet50 and DenseNet121 across a large hyperparameter space. Using hyperparameter optimization, each of the three models was trained on 400 sets of hyperparameters suggested by the HyperSpace search algorithm. The CrossedWires dataset includes PyTorch and Tensorflow models with test accuracies as different as 0.681 on syntactically equivalent models and identical hyperparameter choices. The 340 GB dataset and benchmarks presented here include the performance statistics, training curves, and model weights for all 1200 hyperparameter choices, resulting in 2400 total models. The CrossedWires dataset provides an opportunity to study semantic differences between syntactically equivalent models across popular deep learning frameworks. Further, the insights obtained from this study can enable the development of algorithms and tools that improve reliability and reproducibility of deep learning frameworks. The dataset is freely available at https://github.com/maxzvyagin/crossedwires through a Python API and direct download link.

1 Introduction

Deep learning and neural network techniques [Bengio et al., 2021] are ubiquitous within AI applications that are deployed at scale across various domains (speech [Xiong et al., 2017; Saon et al., 2015; Wang and Chen, 2018; Amodei et al., 2016; Huang et al., 2014], language translation [Young et al., 2018b; Vaswani et al., 2018], Bahdanau et al. [2014], self-driving cars [Maqueda et al., 2018; Ramos et al., 2017; Kulkarni et al., 2018], image search and recognition [Krizhevsky et al., 2012; He et al., 2015; Abbas et al., 2021; Sun et al., 2015], information retrieval [Lam et al., 2015; Liu et al., 2015; Yan et al., 2016], etc.). However, the choice of deep learning frameworks and consequently the hardware (or accelerator; e.g., GPU, TPU, data-flow architectures, etc.) platform used to implement, train, and deploy neural network architectures has an immediate impact on their performance. In specific, syntactically equivalent neural network implementations (across deep learning frameworks) can have a large variance in model accuracies despite controlling for architectures, hyperparameter
Figure 1: An overview of the CrossedWires dataset: We studied the problem of syntactically identical models producing different test accuracies using formal publications and informal anecdotal evidence on forums. We built the SpaceRay library for easily parallelizing hyperparameter search using multiple GPU nodes. We performed $O(10^4)$ GPU hours of exploratory runs to determine the sensitive hyperparameters and their ranges. Finally, we created the CrossedWires dataset of 1200 pairs of models and built the Python API for efficiently accessing the dataset.

Given the wide range of applications that deep learning models are being deployed on, including safety-critical systems [Le et al., 2018] [Biondi et al., 2020] [Henne et al., 2020] and scientific/experimental workflows (e.g., as surrogate models [Jiang et al., 2020] [Christensen et al., 2021] [Kashinath et al., 2021] [Jumper et al., 2021] [Townshend et al., 2021]), or optimal experimental design strategies [Cao et al., 2021] [King et al., 1996] [Sparkes et al., 2010]), there is an immediate need to develop datasets that can quantify the intrinsic variability in model performance based on the choice of framework selected alone as well as how this may impact the choice of performance optimization on a specific hardware platform. The end users of deep learning frameworks naturally expect the accuracy of the models to depend only on the model architecture, training algorithm and the choice of hyperparameters. However, as we demonstrate empirically in this paper, the accuracy of neural network models can vary by up to 68.1% based only on the deep learning framework being used (PyTorch [Paszke et al., 2019] or TensorFlow [Abadi et al., 2016]) even when they share the same neural network architecture, optimization algorithms and choice of training hyperparameters. This problem is further exacerbated if other parameters are considered for optimizing performance (e.g., hardware platform, mixed precision training, network compression, etc.) [Thompson et al., 2020].

To address these challenges and enable the community to build reproducible implementation of neural network models across diverse hardware and software platforms, we developed the CrossedWires dataset that allows for a systematic comparison of PyTorch and TensorFlow models. The creation of the dataset will democratize the study of such framework-based semantic differences between neural network models despite syntactically identical network architectures, hyperparameters and optimization algorithms. The contributions from our dataset can be summarized as follows:

- The CrossedWires dataset provides 1200 pairs of neural network models with syntactically identical architectures, training hyperparameters and optimization algorithms but different test accuracies on the CIFAR-10 dataset using three popular computer vision architec-
tures, namely - ResNet50 [He et al., 2016], VGG16 [Simonyan and Zisserman, 2014] and DenseNet121 [Huang et al., 2017]. The accuracies of models differ by up to 68.1%, 45.2% and 45.7% for VGG16, ResNet50 and DenseNet121 respectively.

- The CrossedWires dataset is made accessible using a Python API interface that allows the end user to load a specific model and the metadata about the accuracy of the models as a Python dataframe and a metadata data sheet (see Supplementary Material). This enables end users to analyze models with divergent behaviors without explicitly downloading the 340GB data that describes all the weights. Our dataset allows for extreme ease of use across the board, needing no more than a few lines of code from installation to neural network initialization with pre-trained weights. In this way, users can access everything from weight and bias vectors, additional model evaluation, and continued training and transfer learning.

- CrossedWires is also a living dataset, where by other users can contribute data and models to study semantic differences between deep learning models. Especially in the context of parameter-rich models (e.g., GPT-3 with 175 billion parameters), such an effort would be needed to reconcile differences and improve performance on various ‘real-world’ tasks.

We feel that the CrossedWires dataset will be useful across multiple fronts. One, for researchers interested in improving reproducibility of deep learning models, the dataset provides a starting point for testing such approaches without the need to extensively train identical networks. With the ability to extend the datasets through a functional API, it will facilitate interactions across disciplines, breaking barriers of communication such that models may be implemented in a more standardized manner, irrespective of hardware/software platforms. Two, it will also enable engineers of novel hardware and software platforms to rigorously test assumptions about model equivalence, starting with the fundamental building blocks of neural networks (e.g., densely connected layers, convolutional layers, etc.). Complementary to community-led efforts such as MLPerf [Mattson et al., 2020], where benchmarking performance across software and hardware platforms have been the primary goal, CrossedWires will enable research in understanding how variability can arise and spur novel research in developing effective interfaces between software and hardware platforms with the primary goal of reproducibility. This will also enable researchers in the area of safety critical systems to quantitatively evaluate and address limitations of deploying models for various application domains. In the context of scientific applications, where surrogate models are being used to accelerate simulation kernels, the variation in model performance as a consequence of hardware and software selections will be valuable to build realistic metrics of confidence in how such models function. Inspired by the approaches developed for scientific simulation toolkits such as molecular dynamics (MD) [Eastman et al., 2017], where simulations instantiated from different MD engines still provide consistent results, CrossedWires will spur the development of better interoperability across software and hardware platforms.

## 2 Methods

### 2.1 Models, Dataset, and Training Details

The CrossedWires dataset comprises of models from hyperparameter optimization runs on three different CNN architectures, namely ResNet50, VGG16 and DenseNet121 that are trained on the CIFAR10 dataset. The primary goal of these searches is to explore the difference in accuracy of syntactically identical models and create a survey-type global overview of the hyperparameter space. Each search is orchestrated using our Python package SpaceRay, resulting in the following artifacts: (i) 2400 total models (1200 each of PyTorch and TensorFlow), (ii) CSV files generated by RayTune [Liaw et al., 2018] on the metrics of each trial, and (iii) pickled Python files containing scipy [Virtanen et al., 2020] OptimizeResult objects which detail the optimization history of the Gaussian process guided search. All the models and the metadata generated during the search process are included in the CrossedWires dataset.

Ease of use was a key design consideration in developing the dataset. Without the ability to integrate into existing codebase or a simple way to retrieve a trained network which works “out of the box”, potential insights could be lost. All objects, including all trained TensorFlow and PyTorch models, may be accessed using the Python API which makes up CrossedWires module. Details on installation and interaction may be found as part of the repository [https://github.com/maxzvyagin/crossedwires](https://github.com/maxzvyagin/crossedwires) and an associated comprehensive documentation site.
The entire dataset can also be downloaded as a single archive [https://storage.googleapis.com/crossed-wires-dataset/full_cifar10_results.zip](https://storage.googleapis.com/crossed-wires-dataset/full_cifar10_results.zip). However, the majority of users will likely benefit more from programmatic access versus an en masse download.

Our experiments focused on the characteristic deep learning problem of image classification, using three well-known convolution neural network architectures: VGG16 [Simonyan and Zisserman, 2014], ResNet50 [He et al., 2016], and DenseNet121 [Huang et al., 2017]. All models were loaded from pre-existing definitions as part of the PyTorch and TensorFlow libraries, with default weight initialization. Importantly, the PyTorch library version of VGG16 had an extra layer of adaptive pooling included to stabilize the gradients which added approximately an extra 100 million parameters when compared to the TensorFlow version. This layer was removed in order to keep the network definitions consistent – the updated PyTorch model definition is included in our repository. The library defined models were selected due to their likelihood of use in common machine learning scenarios, in contrast to potential users writing the code for the entire network from scratch.

The well-known dataset CIFAR10 [Krizhevsky et al.] was selected for this benchmarking experiment, allowing for a moderate level of challenge while simultaneously not requiring immense computational resources. The standard training and test splits were loaded using the PyTorch and TensorFlow libraries, which included 50,000 training samples and 10,000 testing samples. Shuffling was turned off and data values normalized between the values of 0 and 1. Categorical cross entropy was used as the loss function, and the random seed was set to 0. The model implementations and training scripts are available at [https://github.com/maxzvyagin/cross_framework_hpo](https://github.com/maxzvyagin/cross_framework_hpo).

### 2.2 Hyperparameter Optimization

In order to effectively expose the largest divergence of the two different deep learning frameworks, a methodical hyperparameter optimization search strategy was used. The objective function used in the optimization attempted to maximize the absolute value of the difference between the PyTorch and TensorFlow test set accuracy metrics. Four different hyperparameters were tuned - learning rate, batch size, total training epochs, and the epsilon parameter in the Adam optimizer. A relatively wide range for these parameters was fed into the HPO algorithm in order to ensure an exhaustive search. These bounds are shown in Table 1.

| Hyperparameter | Min   | Max   |
|----------------|-------|-------|
| Learning Rate  | $1e^{-8}$ | 0.1   |
| Epochs         | 1     | 50    |
| Adam Epsilon   | $1e^{-8}$ | 1.0   |
| Batch Size     | 10    | 10,000|

We used the approach outlined in the HyperSpace hyperparameter optimization library to examine the optimal settings for the various deep learning networks. The experiments reported here tuned the 4 hyperparameters, leading to $(2^4 = 16)$ hyperparameter spaces being fed into scikit-optimize, with an overlap factor $\phi = 0.5$. Our implementation is a more automated and user friendly extension of the hyperparameter search defined in the original HyperSpace implementation [Young, 2017]. As demonstrated previously, HyperSpace can discover hyperparameter settings that can outperform other approaches and result in optimal settings for a model’s performance [Young et al., 2018a, 2020].

These individual spaces are then fed into the Ray Tune SkOptSearch implementation, which integrates with the scikit-optimize Gaussian process search algorithm to optimize within each hyperparameter space and evaluates them in parallel. This entire process is handled by the SpaceRay library ([www.github.com/maxzvyagin/spaceray](https://www.github.com/maxzvyagin/spaceray)). For each generated scikit-optimize search space, 25 trials were performed, for a total of 400 tested hyperparameter sets per neural network architecture. For each architecture, this then translates to 800 sets of model weights (400 PyTorch, 400 TensorFlow), for a total of 2400 model weights and 1200 tested hyperparameter configurations. All trials were logged using Weights and Biases [Biewald, 2020] and the links to these logs are included in the documentation and the supplementary material. In addition, the CSV file exports of the Weights and Biases logs are directly included as a part of the CrossedWires dataset.

[https://pytorch.org/vision/stable/_modules/torchvision/models/vgg.html#vgg16](https://pytorch.org/vision/stable/_modules/torchvision/models/vgg.html#vgg16)
2.3 Hardware and Environment Details

The exploratory runs as well as the dataset generation experiments were performed on the Lambda system at Argonne National Laboratory. Each node in the Lambda system has 8 NVIDIA Tesla V100 GPUs and 80 Intel Xeon Gold 6148 CPUs. The system utilized NVIDIA driver version 470.57.02, and CUDA version 11.4. Each trial was automatically allocated a single GPU and CPU by RayTune. While replication of the dataset will only require approximately $O(10^2)$ GPU-hours, our exploratory studies to determine the sensitive hyperparameters and parameter regimes took $O(10^4 - 10^5)$ GPU-hours.

3 Benchmark Results and Dataset Observations

3.1 Distribution of Results

As expected, there is a wide range in the final accuracy metrics for both TensorFlow and PyTorch, in addition to a surprisingly wide range of total divergence between the two frameworks, depending on the selected hyperparameter settings. The distributions of the individual accuracy and accuracy difference metrics are displayed in Figure 2. Overall, we see that the majority of the HPO trials generate high test set accuracy in both frameworks, despite the accuracy distribution not being exactly the same. Noticeably, PyTorch has a greater overall density at the top end of the accuracy spectrum across all three architectures. In addition, we see that the majority of the accuracy difference distributions (green line) are at or around zero, with a markedly higher density of non-zero trials in the DenseNet architecture (Figure 2c). From these plots, it is clear that all three HPO searches contain trials with a non-trivial accuracy difference between PyTorch and TensorFlow models of above 5%. Overall, 52.3% of the trials that make up the dataset resulted in a model pair which diverges by at least 5%.

Table 2: Statistical summary of the accuracy difference metric for each tested architecture.

| Architecture | Min             | Max     | Median  | Mean  |
|--------------|-----------------|---------|---------|-------|
| VGG          | $4.17 \times 10^{-10}$ | 0.681   | 0.0843  | 0.123 |
| ResNet       | $1.36 \times e^{-4}$ | 0.452   | 0.0418  | 0.0779|
| DenseNet     | $2.17 \times e^{-4}$ | 0.457   | 0.0563  | 0.104 |

Within each architecture, there are a range of hyperparameter configurations which lead to high accuracy in both frameworks, those which lead to low accuracy in both frameworks, those which lead to high PyTorch accuracy but low TensorFlow accuracy, and vice versa. Unsurprisingly, the final accuracy statistics, including divergence between the frameworks, varies based on the network architecture. The range of the test set accuracy for each individual framework does not necessarily have a linear relationship with the number of parameters within the network. Interestingly, the lowest TensorFlow accuracy in DenseNet is zero, while it is non-zero for the other two architectures (Table 3).
Table 3: Statistical summary of individual framework accuracy on the test dataset, for both PyTorch (PT) and TensorFlow (TF).

| Architecture | PT Min | TF Min | PT Max | TF Max |
|--------------|--------|--------|--------|--------|
| VGG          | 0.0959 | 0.100  | 0.786  | 0.796  |
| ResNet       | 0.0978 | 0.0493 | 0.699  | 0.671  |
| DenseNet     | 0.0799 | 0.0    | 0.764  | 0.771  |

Table 4: Top three and bottom three sets of hyperparameter results for VGG architecture when sorted by accuracy difference.

| Adam Epsilon | Batch Size | Learning Rate | Epochs | PT Test Acc | TF Test Acc | Accuracy Diff |
|--------------|------------|---------------|--------|-------------|-------------|---------------|
| 0.19658      | 202        | 0.09901       | 50     | 0.09998     | 0.78150     | 0.68152       |
| 0.73954      | 22         | 0.06213       | 21     | 0.75619     | 0.10000     | 0.65619       |
| 0.16867      | 242        | 0.09234       | 21     | 0.75329     | 0.10000     | 0.65329       |
| 0.84102      | 10         | 0.05205       | 21     | 0.10000     | 0.10000     | 0.00000       |
| 0.07937      | 10         | 0.04891       | 7      | 0.10000     | 0.10000     | 0.00000       |
| 0.35535      | 10         | 0.04866       | 46     | 0.10000     | 0.10000     | 0.00000       |

Overall, the VGG architecture has the greatest level of maximum model divergence at 68.1%, with the maximum in ResNet and DenseNet architectures being about 23% less (Table 2). Notably, although the individual framework statistics are similar for VGG and DenseNet, the maximum accuracy divergence is 20% higher in VGG. In other words, the top trials of the VGG architecture results in Table 4 generate models where one framework reaches a performance level similar to the individual maximums seen in Table 3. However, in the DenseNet architecture results in Table 6, even the high performing network in the top trials falls short of the 76-77% maximum performance level (Table 5). This is a key result, as it is then plausible that a top performing set of hyperparameters for VGG (selected using a single framework search as is normally done) could be unstable in the other framework. In DenseNet, on the other hand, this is not the case, as the top “divergent” parameter configurations do not lead to maximum performance in either framework. The same holds true for the ResNet architecture, with the individual framework accuracies in Table 5 showing a maximum potential accuracy of 61% in an individual framework, while in Table 3 the maximum potential accuracy is 69%. All trial results for the three architectures can be found in the supplementary material and as part of the hosted dataset.

Table 5: Top three and bottom three sets of hyperparameter results for ResNet architecture when sorted by accuracy difference.

| Adam Epsilon | Batch Size | Learning Rate | Epochs | PT Test Acc | TF Test Acc | Accuracy Diff |
|--------------|------------|---------------|--------|-------------|-------------|---------------|
| 0.20390      | 382        | 0.05596       | 26     | 0.59364     | 0.09990     | 0.49374       |
| 0.20259      | 466        | 0.05103       | 24     | 0.61146     | 0.12910     | 0.48236       |
| 0.46381      | 502        | 0.07989       | 20     | 0.57465     | 0.10610     | 0.46855       |
| 0.53622      | 904        | 0.03705       | 26     | 0.47656     | 0.47680     | 0.00024       |
| 0.18580      | 388        | 0.01245       | 20     | 0.53219     | 0.53240     | 0.00021       |
| 0.91122      | 904        | 0.07455       | 45     | 0.53747     | 0.53730     | 0.00017       |

3.2 Hyperparameter Space Topology

Through Figures 3 and 4, it is clear that the hyperparameter configurations leading to divergent results between PyTorch and Tensorflow are not homogeneous across the different network architectures. In Figure 3, the 4D hyperparameter space is visualized against the top 50% of accuracy difference results (bottom 50% are colored in gray), painted by the level of accuracy difference. The distribution of these points appears to be unique to each individual architecture without any clear regions of similarity across the three architectures. However, there does appear to be some clustering: for example, in the DenseNet figure 3, there is a clear cluster in the very center of the axes of an ~ 0.4 accuracy difference, with turquoise colored points. The greatest variation in the hyperparameter
Table 6: Top three and bottom three sets of hyperparameter results for DenseNet architecture when sorted by accuracy difference.

| Adam Epsilon | Batch Size | Learning Rate | Epochs | PT Test Acc | TF Test Acc | Accuracy Diff |
|--------------|------------|---------------|--------|-------------|-------------|---------------|
| 0.37500      | 589        | 0.05955       | 2      | 0.54946     | 0.11050     | 0.43896       |
| 0.62937      | 824        | 0.08118       | 2      | 0.52159     | 0.08830     | 0.43329       |
| 0.37500      | 686        | 0.06250       | 3      | 0.56427     | 0.15010     | 0.41417       |
| 0.08772      | 602        | 0.02302       | 46     | 0.73392     | 0.73320     | 0.00072       |
| 0.71086      | 370        | 0.08254       | 43     | 0.71602     | 0.71650     | 0.00048       |
| 0.60260      | 13         | 0.05400       | 1      | 0.09990     | 0.10000     | 0.00010       |

Figure 3: Visualization of hyperparameter space with respect to accuracy difference between PyTorch and TensorFlow. Size of points corresponds to epsilon parameter of Adam. Points are painted if above threshold of median accuracy difference. Median statistics can be found in Table 2. (a) corresponds to VGG16, (b) corresponds to ResNet50, and (c) corresponds to DenseNet121.

topology of the painted points does seem to be in the VGG model results (Figure 3a) - there are some small clusters present, however, the majority of the points are distributed somewhat evenly across the entire visualized hyperparameter space.

By calculating the mutual information between the hyperparameter settings and the final accuracy difference between the two frameworks, it is possible to infer the importance and impact of each individual hyperparameter setting on divergence of the resulting models. Both univariate and bivariate results were computed, to understand the effect of both individual and pairwise sets of the hyperparameters. This analysis is presented in Figure 4. From this, we see that the Adam epsilon parameter has the highest influence on the final accuracy difference in the VGG architecture, the pair of epochs and Adam epsilon has the highest influence in ResNet, and the epochs parameters has the highest influence in DenseNet. This is a key understanding: it shows that architecture must be considered when attempting to create stable, framework agnostic hyperparameter settings. This plot also demonstrates that different categories of hyperparameter settings must not be discounted when a novel architecture is involved. For example, the Adam epsilon parameter is not of particularly high importance in the DenseNet architecture, but it is the maximally important parameter in VGG. If this hyperparameter search-based experiment was only performed on DenseNet, with the intent to extrapolate these results, one could erroneously conclude that the epsilon value could instead be hardcoded in hyperparameter searches for subsequent architectures such as VGG. Further, the relatively high values of mutual information found within the bivariate computations show that hyperparameters should not only be considered in isolation.

Another advantage of using our hyperparameter optimization strategy is that it enables one to examine the partial dependency of the hyperparameters and its impact on model performance (see supplementary material, partial dependency plots). Given that very few settings of hyperparameters actually end up ‘sampling’ good model performance (i.e., accuracy), understanding the innate structure of the hyperparameter space can be valuable in fine tuning the models across different frameworks. While this represents just a snapshot of the 4-dimensional landscape (spanned by the hyperparameters), complex models can include higher-order dependencies that may need principled approaches to characterize the overall performance space of semantic equivalence. Such insights are enabled within our dataset implicitly via our data API and SpaceRay.
Figure 4: Mutual information between hyperparameter settings (individual and pairwise) and accuracy difference. All hyperparameter settings and mutual information values were normalized between 0 and 1, then digitized with bin sizes of 0.1 [Harris et al., 2020]. Univariate and bivariate values have been calculated. Both orders of the bivariate data were computed, with the average taken as the final result. To address the non-deterministic nature of this calculation, the computation was repeated 50 times - the mean and standard deviation are shown here. Mutual information was calculated using the NPEET library [Ver Steeg].

4 Related Work

Machine learning benchmarks Benchmarking is a key area of interest to the machine learning community, allowing for effective tracking, collective knowledge, and state of the art performance. An example of this kind of collection is MLPerf, a benchmarking suite which is used to measure and record the performance of deep learning networks on various hardware systems [Mattson et al., 2020]. This organization of knowledge is key in keeping the industry moving forward in pursuit of continuously accelerating training and inference times. Another example is the Papers with Code website, which aggregates accuracy metrics on different architectures and datasets, showcasing which submissions are currently state of the art and linking the statistics to the relevant papers and repositories [PWC]. However, to our knowledge there is very little data in understanding how model performance can vary as a consequence of the choice of a particular framework, hyperparameter settings and how the model is consequently optimized and deployed.

In this paper, we focus on two of the most popular deep learning frameworks, PyTorch and TensorFlow. Both frameworks implement the sets of kernels, layers, and operations required to realize neural networks, however, they do so in significantly different ways. PyTorch is imperative and based on dynamic computation [Paszke et al., 2019]. TensorFlow, on the other hand, is graph-based, allows for kernel substitution at runtime, and is automatically tuned for specific hardware based on resource allocation [Abadi et al., 2016]. There are also noted differences in certain mathematical operation implementations such as the convolution and optimization algorithms. Both of them leverage the cuDNN library [Chetlur et al., 2014], a set of primitives used to accelerate graphics processing unit (GPU) computation. Peer reviewed sources do exist which compare hardware performance between PyTorch and TensorFlow, such as in [Jain et al., 2019] which performed a review of deep networks on modern CPU clusters.

Common Representation of machine learning models At this time, translation between deep learning frameworks can be cumbersome. One potential solution to this has been the introduction of the Open Neural Network Exchange (ONNX) [Bai et al., 2019], which attempts to address framework translation by defining a separate intermediate representation. Although widely adopted for its ease of representation, translating larger and more complex deep learning models and specific aspects (perhaps unique to an implementation framework or hardware) can be challenging to capture within its description. Other problems include translation of the architecture and layers which make up the network, and the translation of operations such as custom training loops. This also does not account for the potential that inference mechanisms could vary between frameworks. Often, the path of least resistance is to simply re-train in a new framework, however, this comes with its own challenges,
of which hyperparameter optimization is just one. We posit that by co-training two syntactically equivalent networks across different implementation frameworks, one can obtain valuable insights into the nature of affects that hyperparameters may induce on model performance within a unified evaluation framework. The CrossWire dataset provides a starting point for such evaluations.

5 Conclusions

In this paper, we have presented the initial generation and statistical characterization of a dataset which will allow for improved understanding of the differences between deep learning framework implementations. Our dataset could prove to be highly useful to better understand the dependence of model implementation in the context of complex hyperparameter spaces which eventually plays an essential role in its deployment and successful application. By providing this dataset to the machine learning community, we hope to provide researchers with the key to unlock novel approaches that improve the stability of machine learning models, and more importantly to develop a rational understanding of how to approach hyperparameter settings. Ideally, this dataset will allow for generalizable insights that will make way for informed and stable hyperparameter configuration without requiring extreme levels of compute power and extensive hyperparameter searches.

It is important to note that while this dataset only consists of the three models as applied to the CIFAR-10 dataset, a significant number of other models (e.g., multi-layer perceptron, Alexnet [Krizhevsky et al., 2012], etc.) and datasets were explored (including Fashion-MNIST [Xiao et al., 2017], ImageNet [Deng et al., 2009], etc.) were explored. In addition, the approach presented here is not limited to only computer vision models and can be extended to complex models (for e.g., language models such as BERT [Devlin et al., 2018], GPT [Radford et al., 2019]) and other scientific datasets. Further, in the context of exploring complex hyperparameter spaces, we deliberately chose to examine a 4-dimensional space. This was a practical choice, rather than a limitation of the hyperparameter optimization approach since larger space exploration would necessarily need extensive computational resources as well. Given the opportunity to expand this dataset, we will gladly incorporate larger models and hyperparameter spaces. We hope that as a living dataset, our efforts will continue to evolve and involve the broader scientific community in contributing to our dataset and enable better development of reproducible deep learning models. This also reflects on how important it would be to quantify the inter- and intra-framework variability when implementing foundational models for AI [Bommasani et al., 2021].

This contribution to the machine learning community must be a living dataset in order to realize its full potential and provide the greatest level of utility. We invite submissions to the dataset, with the hope of expanding our knowledge base to other machine learning frameworks, datasets, architectures, and hardware systems. Submissions must be formatted and include all code in order to be considered as a contribution, in addition to following standard reproducibility guidelines. Details for contribution are included in the documentation, and will take the form of a GitHub pull request which maintains the streamlined API structure.

Acknowledgments and Disclosure of Funding

Funding for this work was provided by the Department of Energy’s Advanced Scientific Computing Research Program through grant number 31975.2 to Argonne National Laboratory for the Co-Design of Advanced Artificial Intelligence (AI) Systems for Predicting Behavior of Complex Systems Using Multimodal Datasets project. The research was partially supported by the National Science Foundation SPX award #1822976, National Science Foundation award #2113307, DARPA GARD contract #HR00112020002, and ONR Science of AI program grant #N00014-21-1-2332. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

References

Papers with Code - The latest in Machine Learning. URL https://paperswithcode.com/

Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, et al. Tensorflow: A system for large-scale
machine learning. In 12th USENIX symposium on operating systems design and implementation (OSDI), pages 265–283. 2016.

Asmaa Abbas, Mohammed M Abdelsamea, and Mohamed Medhat Gaber. Classification of covid-19 in chest x-ray images using detrac deep convolutional neural network. Applied Intelligence, 51(2):854–864, 2021.

Dario Amodei, Sundaram Ananthanarayanan, Rishita Anubhai, Jingliang Bai, Eric Battenberg, Carl Case, Jared Casper, Bryan Catanzaro, Qiang Cheng, Guoliang Chen, et al. Deep speech 2: End-to-end speech recognition in english and mandarin. In International conference on machine learning, pages 173–182. PMLR, 2016.

Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. Neural machine translation by jointly learning to align and translate. arXiv preprint arXiv:1409.0473, 2014.

Junjie Bai, Fang Lu, Ke Zhang, et al. Onnx: Open neural network exchange. https://github.com/onnx/onnx, 2019.

Yoshua Bengio, Yann Lecun, and Geoffrey Hinton. Deep learning for ai. Commun. ACM, 64(7):58–65, June 2021. ISSN 0001-0782. doi: 10.1145/3448250. URL https://doi.org/10.1145/3448250

Lukas Biewald. Experiment tracking with weights and biases, 2020. URL https://www.wandb.com/. Software available from wandb.com.

Alessandro Biondi, Federico Nesti, Giorgiomaria Cicero, Daniel Casini, and Giorgio Buttazzo. A safe, secure, and predictable software architecture for deep learning in safety-critical systems. IEEE Embedded Systems Letters, 12(3):78–82, 2020. doi: 10.1109/LES.2019.2953253.

Rishi Bommasani, Drew A Hudson, Ehsan Adeli, Russ Altman, Simran Arora, Sydney von Arx, Michael S Bernstein, Jeannette Bohg, Antoine Bosselut, Emma Brunskill, et al. On the opportunities and risks of foundation models. arXiv preprint arXiv:2108.07258, 2021.

Liwei Cao, Danilo Russo, Kobi Felton, Daniel Salley, Abhishek Sharma, Graham Keenan, Werner Mauer, Huanhuan Gao, Leroy Cronin, and Alexei A. Lapkin. Optimization of formulations using robotic experiments driven by machine learning doe. Cell Reports Physical Science, 2(1):100295, 2021. ISSN 2666-3864. doi: https://doi.org/10.1016/j.xcrp.2020.100295. URL https://www.sciencedirect.com/science/article/pii/S2666386420303210

Sharan Chetlur, Cliff Woolley, Philippe Vandermersch, Jonathan Cohen, John Tran, Bryan Catanzaro, and Evan Shelhamer. cudnn: Efficient primitives for deep learning. arXiv preprint arXiv:1410.0759, 2014.

Anders S. Christensen, Sai Krishna Sirumalla, Zhuoran Qiao, Michael B. O’Connor, Daniel G. A. Smith, Feizhi Ding, Peter J. Bygrave, Animashree Anandkumar, Matthew Welborn, Frederick R. Manby, and Thomas F. Miller III au2. Orbnet denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and dft accuracy, 2021.

Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In 2009 IEEE conference on computer vision and pattern recognition, pages 248–255. Ieee, 2009.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv preprint arXiv:1810.04805, 2018.

Peter Eastman, Jason Swails, John D. Chodera, Robert T. McGibbon, Yutong Zhao, Kyle A. Beauchamp, Lee-Ping Wang, Andrew C. Simmonett, Matthew P. Harrigan, Chaya D. Stern, Rafal P. Wiewiora, Bernard R. Brooks, and Vijay S. Pande. Openmm 7: Rapid development of high performance algorithms for molecular dynamics. PLOS Computational Biology, 13(7):1–17, 07 2017. doi: 10.1371/journal.pcbi.1005659. URL https://doi.org/10.1371/journal.pcbi.1005659

Timnit Gebru, Jamie Morgenstern, Briana Vecchione, Jennifer Wortman Vaughan, Hanna Wallach, Hal Daumé III au2, and Kate Crawford. Datasheets for datasets, 2020.
GitHubIssue. Tensorflow codes totally different result with pytorch’s issue 7624 tensorflow/tensorflow. URL https://github.com/tensorflow/tensorflow/issues/7624

GitHubIssue#2. Low validation accuracy of the converted pytorch model from tensorflow issue 520 microsoft/mmdnn. URL https://github.com/Microsoft/MMdnn/issues/520

Charles R. Harris, K. Jarrod Millman, Stéfan J. van der Walt, Ralf Gommers, Pauli Virtanen, David Cournapeau, Eric Wieser, Julian Taylor, Sebastian Berg, Nathaniel J. Smith, Robert Kern, Matti Picus, Stephan Hoyer, Marten H. van Kerkwijk, Matthew Brett, Allan Haldane, Jaime Fernández del Río, Mark Wiebe, Pearu Peterson, Pierre Gérard-Marchant, Kevin Sheppard, Tyler Reddy, Warren Weckesser, Hameer Abbasi, Christoph Gohlke, and Travis E. Oliphant. Array programming with NumPy. Nature, 585(7825):357–362, September 2020. doi: 10.1038/s41586-020-2649-2. URL https://doi.org/10.1038/s41586-020-2649-2

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In Proceedings of the IEEE international conference on computer vision, pages 1026–1034, 2015.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 770–778, 2016.

Maximilian Henne, Adrian Schwaiger, Karsten Roscher, and Gereon Weiss. Benchmarking uncertainty estimation methods for deep learning with safety-related metrics. In SafeAI@ AAAI, pages 83–90, 2020.

Gao Huang, Zhuang Liu, Laurens Van Der Maaten, and Kilian Q Weinberger. Densely connected convolutional networks. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 4700–4708, 2017.

Po-Sen Huang, Minje Kim, Mark Hasegawa-Johnson, and Paris Smaragdis. Deep learning for monaural speech separation. In 2014 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), pages 1562–1566. IEEE, 2014.

Arpan Jain, Ammar Ahmad Awan, Quentin Anthony, Hari Subramoni, and Dhabaleswar K. DK Panda. Performance characterization of dnn training using tensorflow and pytorch on modern clusters. In 2019 IEEE International Conference on Cluster Computing (CLUSTER), pages 1–11, 2019. doi: 10.1109/CLUSTER.2019.8891042.

Chiyu “Max” Jiang, Soheil Esmaeilzadeh, Kamyar Azizzadenesheli, Karthik Kashinath, Mustafa Mustafa, Hamdi A. Tchelepi, Philip Marcus, Mr Prabhat, and Anima Anandkumar. Mesh-freeflownet: A physics-constrained deep continuous space-time super-resolution framework. In SC20: International Conference for High Performance Computing, Networking, Storage and Analysis, pages 1–15, 2020. doi: 10.1109/SC41405.2020.00013.

John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, et al. Highly accurate protein structure prediction with alphafold. Nature, pages 1–11, 2021.

K Kashinath, M Mustafa, A Albert, JL Wu, C Jiang, S Esmaeilzadeh, K Azizzadenesheli, R Wang, A Chattopadhyay, A Singh, et al. Physics-informed machine learning: case studies for weather and climate modelling. Philosophical Transactions of the Royal Society A, 379(2194):20200093, 2021.

Ross D King, Stephen H Muggleton, Ashwin Srinivasan, and MJ Sternberg. Structure-activity relationships derived by machine learning: The use of atoms and their bond connectivities to predict mutagenicity by inductive logic programming. Proceedings of the National Academy of Sciences, 93(1):438–442, 1996.

Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton. Cifar-10 (canadian institute for advanced research). URL http://www.cs.toronto.edu/~kriz/cifar.html

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. Advances in neural information processing systems, 25:1097–1105, 2012.
Ruturaj Kulkarni, Shruti Dhavalikar, and Sonal Bangar. Traffic light detection and recognition for self driving cars using deep learning. In 2018 Fourth International Conference on Computing Communication Control and Automation (ICCCBEA), pages 1–4. IEEE, 2018.

An Ngoc Lam, Anh Tuan Nguyen, Hoan Anh Nguyen, and Tien N Nguyen. Combining deep learning with information retrieval to localize buggy files for bug reports (n). In 2015 30th IEEE/ACM International Conference on Automated Software Engineering (ASE), pages 476–481. IEEE, 2015.

Michael Truong Le, Frederik Diehl, Thomas Brunner, and Alois Knol. Uncertainty estimation for deep neural object detectors in safety-critical applications. In 2018 21st International Conference on Intelligent Transportation Systems (ITSC), pages 3873–3878, 2018. doi: 10.1109/ITSC.2018.8569637.

Richard Liaw, Eric Liang, Robert Nishihiara, Philipp Moritz, Joseph E Gonzalez, and Ion Stoica. Tune: A research platform for distributed model selection and training. arXiv preprint arXiv:1807.05118, 2018.

Xiaodong Liu, Jianfeng Gao, Xiaodong He, Li Deng, Kevin Duh, and Ye-Yi Wang. Representation learning using multi-task deep neural networks for semantic classification and information retrieval. 2015.

Ana I Maqueda, Antonio Loquercio, Guillermo Gallego, Narciso García, and Davide Scaramuzza. Event-based vision meets deep learning on steering prediction for self-driving cars. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pages 5419–5427, 2018.

Peter Mattson, Vijay Janapa Reddi, Christine Cheng, Cody Coleman, Greg Diamos, David Kanter, Paulius Micikevicius, David Patterson, Guenther Schmuelling, Hanlin Tang, Gu-Yeon Wei, and Carole-Jean Wu. Mlperf: An industry standard benchmark suite for machine learning performance. IEEE Micro, 40(2):8–16, 2020. doi: 10.1109/MM.2020.2974843.

Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Kopf, Edward Yang, Zachary DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. Pytorch: An imperative style, high-performance deep learning library. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 32, pages 8026–8037. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper/2019/file/bdbca288fee7f92f2bfa9f7012727740-Paper.pdf.

PyTorchDiscuss. Pytorch vs tensorflow gives different results. URL https://discuss.pytorch.org/t/pytorch-vs-tensorflow-gives-different-results/4630.

Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, Ilya Sutskever, et al. Language models are unsupervised multitask learners. OpenAI blog, 1(8):9, 2019.

Sebastian Ramos, Stefan Gehrig, Peter Pinggera, UweFranke, and Carsten Rother. Detecting unexpected obstacles for self-driving cars: Fusing deep learning and geometric modeling. In 2017 IEEE Intelligent Vehicles Symposium (IV), pages 1025–1032. IEEE, 2017.

Félix Renard, Soulaimane Guedria, Noel De Palma, and Nicolas Vuillerme. Variability and reproducibility in deep learning for medical image segmentation. Scientific Reports, 10(1):1–16, 2020.

George Saon, Hong-Kwang J Kuo, Steven Rennie, and Michael Picheny. The ibm 2015 english conversational telephone speech recognition system. arXiv preprint arXiv:1505.05899, 2015.

Karen Simonyan and Andrew Zisserman. Very deep convolutional networks for large-scale image recognition. arXiv preprint arXiv:1409.1556, 2014.

Andrew Sparkes, Wayne Aubrey, Emma Byrne, Amanda Clare, Muhammad N Khan, Maria Liakata, Magdalena Markham, Jem Rowland, Larisa N Soldatova, Kenneth E Whelan, et al. Towards robot scientists for autonomous scientific discovery. Automated Experimentation, 2(1):1–11, 2010.
