TensorX: Extensible API for Neural Network Model Design and Deployment

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Abstract

TensorX is a Python library for prototyping, design, and deployment of complex neural network models in TensorFlow. A special emphasis is put on ease of use, performance, and API consistency. It aims to make available high-level components like neural network layers that are, in effect, stateful functions, easy to compose and reuse. Its architecture allows for the expression of patterns commonly found when building neural network models either on research or industrial settings. Incorporating ideas from several other deep learning libraries, it makes it easy to use components commonly found in state-of-the-art models. The library design mixes functional dataflow computation graphs with object-oriented neural network building blocks. TensorX combines the dynamic nature of Python with the high-performance GPU-enabled operations of TensorFlow.

This library has minimal core dependencies (TensorFlow and NumPy) and is distributed under Apache License 2.0 licence, encouraging its use in both an academic and commercial settings. Full documentation, source code, and binaries can be found in https://tensorx.org/.

1 Introduction

Machine Learning has become one of the emerging cornerstones of modern computing. With the availability of both computational power and large amounts of data, artificial neural networks became one of the building blocks of large scale machine learning systems. Graphical Processing Units (GPUs), and dedicated hardware like Tensor Processing Units (TPUs) [14] reignited the interest in large-scale vectorized computations. The performance and architecture of such hardware makes it a perfect choice for operating on data in vectors, matrices, and higher-dimensional arrays. This contributed to the popularity of neural network models which, while theoretically attractive for being universal function approximators, were mostly set aside in the past due to their computational requirements.

Neural networks have been shown to be the state-of-the-art models in a wide variety of tasks from text classification [23] to machine translation [9], or semantic image segmentation [20]. However, replicating existing results can be particularly challenging, not just due to computational requirements or lack of clear experiment specifications, but because reference implementations re-implement software components from scratch. This creates a barrier of entry in many research tasks and makes it difficult to do iterative research. In other words, this problem makes it difficult for the software to support the provenance of reported results [13].

TensorX aims to alleviate this problem by implementing abstractions that are usable in a wide variety of tasks to write high-level code. These components are easy to re-use across different models and make a separation between common deep learning technical problems and experiment definition. (e.g. re-using a recurrent neural network cell to build complex recurrent layers, or embedding lookup layers that handle dynamic input sequences or sparse inputs.) This library is implemented in pure Python and it is written to be a high-level API on top of Tensorflow [1]. Tensorflow is a library that allows expressions to be defined using generalized vector data structures called tensors or high-dimensional arrays, also the core component of the popular NumPy library [10]. Computation graphs written with Tensorflow are transparently transcoded to lower level machine code that can be be optimally executed both in the CPU and GPUs along with TPUs (either in a single machine or in a distributed cluster).

The conceptual workflow of developing and deploying neural network models is simple:

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• gather relevant data in the target domain and design a task such that the domain and/or the task can be captured by a model

• at the training phase, a learner or trainer takes the input data in the form of vectorial features, and outputs the state of a learned model

• at the inference phase, the model takes input features and outputs predictions or decisions, in the case of a controller

• at the evaluation phase, metrics are used to quantify the quality of the trained model

However, each of these components becomes more intricate as we need to regularize models, evaluate training progress and model quality, decide on which architectures to use, reuse complex modules throughout larger architectures, or develop new components to accommodate domain knowledge or inductive bias. For this reason, the ability to quickly prototype, standardize, and distribute reusable components is fundamental to all scenarios, from scientific research to applications in production in the industry.

TensorX, similarly to e.g. Keras [7], aims to be a consistent high-level API to build neural network models in the Python ecosystem. Keras was absorbed into the Tensorflow codebase, departing from its initial multi-backend design. We believe that high-level libraries should be decoupled from the numerical computation backend. Other projects such as pytorch [18] also adopt this position. We believe that this makes the case for faster iterations on bleeding-edge components, making them accessible to the community faster, while the core backend adds operations to its code base based on scientific robustness, and how generalizable or useful these operations are to the community.

The TensorX website contains API documentation, tutorials, and examples showcasing multiple framework features. It also points to the public repository with the source code, and gives instructions on how to install the library. The library source code is distributed under the Apache License 2.0 licence.

1.1 Related Software

A number of high-level deep learning libraries and frameworks have emerged over the years. This sections does not meant to present an exhaustive list of existing libraries but rather a representation of the existing ecosystem. At their core, most low-level libraries share the support for multi-dimensional array transformations, automatic differentiation, and the efficient execution of computation graphs in GPUs or similar hardware. Higher-level libraries, on the other hand, vary in complexity of the operations supported, the number of abstractions dedicated to neural networks in particular, and machine learning in general, and the target domains they intend to support.

Lower-level deep learning libraries include [1], PyTorch [18], Chainer [21], or [6]. More recent additions to deep learning libraries include JAX [5], adding automatic differentiation and GPU support to NumPy [10], along with graph computation optimization using the Accelerated Linear Algebra (XLA) compiler (also used by Tensorflow). Other libraries such as DyNet [17] offer features like dynamic batching [16], particularly useful for domains that involve the encoding of variable-length sequences such as Natural Language Processing. Dynet occupies somewhat a different position in the ecosystem in that it provides both lower level components and higher-level abstractions like Recurrent Neural Networks.

Examples of higher-level APIs and specialised frameworks include: [12], which is built on top of PyTorch and contains high-level components like layer building blocks along with configurable training loops. This perhaps the closest to TensorFlow in terms of scope, albeit for a different backend library; Sonnet [8], with a set of high-level computation building blocks for Tensorflow. TensorFlow is similar to Sonnet in the sense that layers can be used as standalone functions, but additionally, it also includes utilities to build and validate layer graphs, compile those graphs, and integrate them in models that can then be trained and evaluated; TFX [3] augments Tensorflow with components for model deployment and serving; Objax [4], similar to previous frameworks, but built on top of the JAX [5] backend; HuggingFace's Transformers [22], which aims to make a specific neural network architecture accessible to end-users with a library of pre-trained models readily available. This is something TensorFlow considers for future work, but it should be noted that the core library is intended for general purpose use.

Much like other high-level Machine Learning libraries, TensorFlow is built on top of a lower level library, Tensorflow [1] in this case. Tensorflow provides GPU-optimized operations, automatic differentiation, and machine learning oriented components like optimizers. Despite libraries like PyTorch [18] gaining significant popularity due to its simplified imperative programming model, when compared with previous

https://tensorx.org
static computation graph definitions in TensorFlow’s first version, the latest developments in the library led to an adoption of a similar imperative computation graph definition model. We chose to adopt Tensorflow 2 as the core due to its sizeable ecosystem, production-oriented tools, and distributed training capabilities. TensorX doesn’t try to hide Tensorflow functionality but rather extend it and present it in a idiomatic fashion (akin to Sonnet but with added configurable training subroutines). Much like the Keras project [7] (now integrated in the Tensorflow codebase), we intend TensorX to be an API that simplifies neural network rapid prototyping and deployment. We still view such high level component libraries as something that should be developed separately as to provide reusable state-of-the-art components without being dependent on the core library development cycle. Also, separating the core computational components from higher level reusable components makes the code base cleaner.

2 TensorX Overview

TensorX is a library designed specifically for deep learning research. It is built on Tensorflow 2.0 [1], which provides many attractive features for neural network research. The new iteration of Tensorflow (much like PyTorch [18]), provides support for dynamic computation graphs with a clear and imperative "Pythonic" syntax. At the same time, the backend makes the benefits of optimized static computation graphs accessible through automatic compilation of Python functions into Tensorflow graphs. TensorX takes advantage of this and mixes an object-oriented design of stateful neural network layers with layer graphs definitions, these in turn can be compiled into optimized static computation graphs in a transparent fashion for the end-users.

The main library components are illustrated in figure 2. In this section, we will exemplify some of the features of Layer objects and layer Graph utilities. These represent the core design decision behind the library design and set the tone for its usability.

Hyperparameter tuning, model serving, experiment management, along with other kind of high-level tools, while commonly found in various machine learning toolkits, are beyond the scope of the library. The objective of TensorX is to extend the capabilities of Tensorflow as to make research in deep neural networks more productive both in terms of model specification and experiment running, but the library is built with extensibility in mind so that the users can easily contribute to it and integrate it with other tools and libraries.

2.1 Core Components

The core of the library is composed of Layer instances, layer graphs (built automatically by Graph class), and the Module layer which converts multiple layers into a single re-usable component that acts as any other layer. In this section we will give a brief preview of the usage of such components and end with a summary of how these components interact with each other.

Layer At the core neural network building blocks in the TensorX library are Layer objects. Semantically speaking, a layer is an object that can have multiple inputs, an inner state, and a computation function that is applied to its inputs (and depends on the current inner state). Each layer has a single output. In essence, we can say that a Layer instance is a stateful function.
Layer subclasses can range from simple linear transformations (e.g. in the form \( y = Wx + b \) where \( W \) is a weight matrix and \( b \) a vector with biases) to more complex structures used to build recurrent neural networks such as Long short-term memory (LSTM) layers \([11]\) or attention mechanisms \([2]\), or even layers used for regularization such as Dropout \([19]\).

Figure 3 shows an example of basic layer used to construct a computation graph with multiple layers. We can also see how to reuse existing layers in such a way that their internal state is shared between layer instances.

```python
import tensorflow as tf
import tensorx as tx

# stateful input placeholder
x1 = tx.Input(n_units=2)
x1.value = tf.random.uniform([2, 2])

# y = Wx + b
l1 = tx.Linear(x1, n_units=3)
a1 = tx.Activation(l1, tx.relu)
l2 = tx.Linear(a1, n_units=4)
d1 = tx.Dropout(a1, probability=0.4)
l3 = l2.reuse_with(d1)
```

Figure 2: Example with basic layer creation and state re-use. Introducing a regularization layer (Dropout) between layers in another pre-existing graph. Each output is at the same time a layer object and the end-node of a computation graph.

A Layer object is simultaneously a stateful function and the end-node of a computation graph. Executing a layer will execute the entire graph ending in that specific node. If we only want to execute a layer computation on a given set of inputs, we can use the \(\text{compute(*inputs)}\) method. Note also that Input is a special layer that has no inputs, instead, this is used as a stateful placeholder that stores the inputs for the current computation graph.

**Module** A Module is a special utility layer that transforms a computation graph between into a new Layer object. The Module class traces a graph between the given output and its inputs, determine if the graph is valid, and transforms the layers into a single layer/stateful function. A use case for this feature is the development of new TensorX layers, as it allows us to use the state initialization procedure to define complex layer graphs, these can then be transformed into a single module that is executed by the \(\text{compute(*inputs)}\) method. Figure 2 shows an example of Module being used to create a recurrent neural network (RNN) cell.

**Graph** In TensorX, as we have seen previously, by connecting multiple layers to each other, we build layer graphs. These are in effect directed acyclic graphs (DAG) defining a given computation over inputs. To aid with validation and execution of neural network layer graphs, TensorX has a Graph utility class. The Graph class allows for automatic graph construction from output nodes (by recursively visiting each node’s inputs). It also facilitates transversal by dependency ordering along with conversion of arbitrary graphs to functions. Moreover, this conversion allows for TensorX graphs to be compiled in to Tensorflow static computation graphs.

We take advantage of Tensorflow’s graph optimization system to optimize layer graph computations. This system improves the performance of TensorFlow computations through computation graph simplifications and other high-level optimizations. By converting layers into functions that are then trace-compiled into an optimized static graph, we get the best of both worlds (Layer instances are easy to debug in eager mode, and layer graphs are transparently compiled into optimized Tensorflow graphs).

Figure 2.1 shows a summary UML diagram of the previously mentioned components, along with their basic interaction. While there are many ready to use layers in the library, from different types of recurrent neural network cells to sequence lookup, convolution layers among others, this short excerpt illustrates the main design decisions behind the library and set the tone for the usability of the API TensorX provides.
def init_state(self):
    state = super().init_state()
    x = ...
    h = ...
    w = Linear(x, self.n_units, ...)
    u = Linear(h, self.n_units, ...)

    add_wu = Add(w, u)
    output = Activation(add_wu, tx.tanh)

    state.rnn_cell = Module([x, h], output)
    return state

def compute(self, x, *h):
    return self.rnn_cell.compute(x, *h)

Figure 3: Example of recurrent neural network (RNN) cell definition using Module to consolidate a layer graph into a single component that can later be executed.

x1 = Input(n_units=2)
x2 = Input(n_units=4)
l1 = Linear(x1,4)
l2 = Add(l1, x2)
l3 = Linear(l2,2)
g = Graph.build(outputs=l3, inputs=[x1, x2])

fn = g.as_function(compile=True)

Figure 4: Automatic graph building example. The graph g is traced from the output nodes until the inputs are reached. Graphs are also capable of being converted into functions as demonstrated. TensorX uses the dynamic nature of python to create a new function object that can then be traced-compiled by Tensorflow into an optimized static computation graph.

As we can see, layers have access to basic Tensorflow constructs like Tensor, SparseTensor, or Variable, and encapsulate the stateful computations each basic layer provides. Layer states are decoupled from layers as to avoid the need for referencing each layer sharing a given state to propagate a modified member. A Module, as previously discussed, is a special layer that makes use of the Graph utility to encapsulate complex layer graphs as a single reusable object. The graph utility itself is a general data structure that uses only inputs as a transversal method, and a compute method to convert a graph into python function.

For more documentation and examples refer to the library documentation website. The previous are the basic TensorX building blocks used to construct most of the other components (e.g. the training module contains training utilities that make use of Graph instances to encapsulate a model inference, training, and evaluation graphs).

3 Conclusion and Future Work

Deep neural networks continue to play a major role in fields like Natural Language Processing, Computer Vision, Reinforcement Learning, and Machine Learning in general. As these models and methodology continue to gain traction and technology transfer makes them especially attractive to build real-world applications, it is important for model building, and experiment deployment tools to be accessible both in an research, industrial context to end-users. TensorX aims to be an open-source library that fulfils that role allows the community to build upon this work and contribute with relevant components –making state-of-
the-art advancements widely available to everyone without depending on the core development cycle of its backend library Tensorflow.

Future work includes making a set of full models like Transformers readily available using components from the library, full integration with distributed training from Tensorflow and actor-based distributed computing frameworks such as Ray [15]. Finally, our goal is to integrate TensorX with other experiment tracking and monitoring platforms, extending the existing tools to a wider community. TensorX aims to do a couple of things well rather than encapsulating all the possible needs of the Machine Learning community under a single library, as such the goal is to maintain an extendable open platform with solid foundations from which end-users can build.

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