Towards Deep Learning Specification

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Abstract

Deep Learning techniques are applied in software systems rapidly. Therefore, it becomes necessary to specify Deep Learning (DL) application programming interfaces (APIs) for desired output. Unlike traditional software, DL-specific development occupies bugs that exhibit not only crashes but also yield low accuracy and high training time issues. Inspired by the design-by-contract (DbC) methodology, this work proposes a preemptive measure against such bugs, we call it DL Contract. DL Contract aims to document properties of DL libraries and provide developers with a mechanism to prevent low accuracy and high training time-related bugs during development. One of the main challenges towards DL Contract is to specify properties of the training process, which is inaccessible at the functional interface of the DL libraries. Thus, we introduce the notion of ML variable that allows developers to specify the properties of model architecture, data, and training behavior. To evaluate the utility of *DL Contract*, we intend to utilize benchmarks from prior works on DL bug detection and repair after implementing DL Contract for Python-based DL libraries.

CCS Concepts: • Software and its engineering \rightarrow Software notations and tools.

Keywords: Specification, deep learning

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1 Problem

Design by Contract (DbC) [19] improves the reliability of software with precise specifications. The contracts cover mutual obligations (preconditions), benefits (post-conditions), and consistency constraints (invariants) [15]. For traditional

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software approaches like Eiffel [19], JML [16], Spec# [10], Dafny [17] have provided support for writing at the application programming interfaces (API). Those specifications comprise conditions ensured by the client prior to calling the method (*preconditions*), and if the method is called correctly, what it will guarantee (*postconditions*).

Unfortunately, the prevailing DbC methodology, which specifies constraints over the functional interface (formal parameters and return values) of the API methods and fields of the API classes, is not sufficient for documenting deep learning software. In particular, a significant concern is that major DL-specific development issues are related to bugs having accuracy and training time issues. These bugs do not appear as crashes or discrepancies at the functional interface of the DL API. Recent work in software engineering has characterized these bugs, studied fix patterns, and proposed detection and localization strategies. However, there are still research gaps in detecting bugs of DNN models without modifying anything in the client code, importing tools, or instrumenting a model during training. There are several challenges to specify DL libraries, mainly to document clients' code obligations and ensure desired output from the DL software.

2 Motivation

To motivate the need for *DL Contract*, we consider a simple convolution network in Fig. 1 that achieves 99% test accuracy on the MNIST dataset from *Keras* documentation [8]. This DL model is intended to classify images of digits from the MNIST dataset. In this code, MNIST images have been scaled to the [0, 1] range (lines 5-6) and converted to binary class matrices (lines 7-10). After that, at lines 11-19, a Sequential model has been declared with model and layer architecture. The model has been configured for training (line 20) using Compile API, and Fit API (line 22) will train the model.

Fig. 1 shows four different types of bugs that could appear in this model. 1 high dropout rate of *Dropout* API [9] could cause overfitting, i.e., the model fit exactly against its training data. 2 If 'relu' activation function has been used in the last layer (line 19) of Dense API [1, 4, 5]. 3 If loss='binary_crossentropy' (line 20) has been applied as the loss function of Compile API [1, 2, 7]. Lastly, 4 if the data is not normalized before it is fed into the Fit API [5, 6] (lines 5, 6). Any of the above statements could result in bugs yielding low accuracy and high training time. The *Keras* documentation [3] suggests that all of these values are valid for

1

```
(x_train, y_train), (x_test, y_test) = keras.datasets.mnist.load_data()
                                                                                               (x_train, y_train), (x_test, y_test) = keras.datasets.mnist.load_data()
x_train = x_train.astype("float32")/3
x_test = x_test.astype("float32")/25
                                                                                               x_train = x_train.astype("float32"
x_test = x_test.astype("float32")
                                                                                                                                                                                        DL Contract intends to prevent
                                                                                               x_train = np.expand_dims(x_train, -1)
x_test = np.expand_dims(x_test, -1)
x train = np.expand dims(x train, -1)
                                                                                                                                                                                       bugs such as, 1 high dropout
x_test = np.expand_dims(x_test, -1)
y_train = keras.utils.to_categorical(y_train, 18)
                                                                                               y_train = keras.utils.to_categorical(y_train, 10)
                                                                                                                                                                                         rate, 4 data normalization,
y_test = keras.utils.to_categorical(y_test, 10)
                                                                                               y_test = keras.utils.to_categorical(y_test, 10)
   del = keras.Sequential([
keras.Input(shape=(28, 28, 1)),
layers.Conv2D(32, kernel_size=(3, 3), activation="relu"),
                                                                                                 del = keras.Sequential([
keras.Input(shape=(28, 28, 1)),
                                                                                                                                                                                         incorrect last laver activation
                                                                                                                                                                                        function 2, 3 loss function.
                                                                                                        layers.Conv2D(32, kernel_size=(3, 3), activation="relu").
          layers.NaxPooling2D(pool_size=(2, 2)),
layers.NaxPooling2D(pool_size=(3, 3), activation="relu"),
layers.NaxPooling2D(pool_size=(2, 2)),
                                                                                                        layers.NaxPooling20(pool_size=(2, 2)),
layers.NaxPooling20(pool_size=(3, 3), activation="relu"),
layers.MaxPooling20(pool_size=(2, 2)),
                                                                                                                                                                                        Prior work DeepLocalize [22]
                                                                                                        layers.Flatten(),
layers.Dropout(0.8),
layers.Dense(10, activation="relu"),] 2
          lavers.Flatten(),
          layers.Dropout(0.5),
layers.Dense(10, activation="softmax"),])
                                                                                          1
                                                                                                                                                                                       detects 2 ,UMLAUT [21] detects 1
 model.compile(loss="categorical_crossentropy", optimizer="adam",
metrics=["accuracy"])
                                                                                          3
                                                                                                                                                                                       2 AUTOTRAINER [23] detects 4,
                                                                                             model.compile(loss="binary_crossentropy", optimize
                                                                                                               metrics=["accuracy"])
                                                                                         4 model.fit(x_train, y_train, batch_size=128, epochs=15, validation_split=0.1)
                                                                                                                                                                                       NeuraLint [20] can detect only 3
model.fit(x_train, y_train, batch_size=128, epochs=15,
            validation_split=0.1)
score = model.evaluate(x_test, y_test, verbose=8)
                                                                                               score = model.evaluate(x_test, y_test, verbose=0)
  Correct Code (Test Accuracy: ~99%)
                                                                                                  Buggy Code (Test Accuracy: 9.86%)
```

Figure 1. Buggy code (right) [1, 2, 5–7] achieves 9.86% test accuracy, whereas correct code (left) from *Keras* documentation [8] achieves ~ 99% test accuracy. *DL Contract* intends to detect such bugs with informative error messages localizing the bugs.

the respective APIs. Thus, the documentation is still insufficient to prevent such bugs.

To detect such types of bugs in deep learning programs, we propose a technique for applying the concept of *Design* by Contracts [19] to DL APIs. The expert-defined solutions from the Stack Overflow posts, GitHub are considered client code obligations (preconditions). The conditions for better accuracy and training time as the expectation from the DL software are postconditions in our proposed DL Contract mechanism. Prior work, specifically DeepLocalize [22], UM-LAUT [21], AUTOTRAINER [23], and NeuraLint [20] failed to detect all those bugs. DL Contract is not dependent on the model's implementation nor on other debugging techniques like those approaches. DL Contract also does not require any additional compiler or package installation rather, the mechanism of our approach is designed to be embedded on top of Keras APIs by the library developers. DL Contract intends to detect all of these bugs and present the end-users with corrective error messages earlier than previous work.

3 Approach

In order to design and implement *DL Contract*, we need to expose meta-level properties of the deep learning training process and deep learning model structure as variables, which we call *ML variable*. Using *DL Contract* with the help of *ML variable*, developers can specify various properties, including expectations about the model structure, to prevent accuracy and training time related bugs. *DL Contract* enables library developers to write contracts on DL library APIs using annotation based approach with @contract utilizing the notion of model abstraction and *ML variable*. Thus, those contracts need to facilitate end-users of run time assertion checking on the model, data, and training properties at different program points, e.g., before and after model compilation or during training deep learning models.

For instance, when training a DNN with ReLu as the activation function, the gradients of a large percentage of the neurons are zero, and the training accuracy is low [23]. To

specify this, 'zero_gradients_percentage' (percentage of neurons whose gradients is 0 in recent iterations) *ML variable* is utilized. Thus, we can capture properties of hidden layers' activation functions and corresponding training problems by writing the following contract on *Keras* Fit API.

```
1 | @contract(context = 'hidden_layers',activation!='relu',
    zero_gradients_percentage ≤ λ, accuracy ≤ θ)
2 | def fit(self, x=None, y=None,...):
```

Developers can specify by λ and θ thresholds so that training can happen without dying ReLu [23] problem and expected accuracy. In case of a contract violation during training, following message can be shown to the end-users,

```
| Contract violation for Model:fit(). zero_gradients_percentage of 12.07 caused dying relu problem, activation function should not be relu.
```

Next, we describe the technical challenges for design and implement *DL Contract* and how we plan to address them.

Context and *ML variable***:** To apply DbC for deep learning APIs, it is necessary to have additional variables that could capture model abstraction and training behavior. Standard precondition and postcondition contracts are enforced on values of the formal parameters and return values of an API method on the attributes of an API class. Therefore, we introduce context and *ML variable* to specify the model abstraction, its data properties, and training behavior.

DL Contract Runtime Assertion: The traditional assertion technique works on code-level, whereas our proposed *DL Contract* provides model abstraction and exposes *ML variable*. Unlike a traditional contract checker, the *DL Contract* must be aware of context and *ML variable*. By using the model abstraction and *ML variable*, *DL Contract* enables library developers to annotate *Keras* APIs. Thus, it benefits end-users to check their model, data, and training properties at different program points. For instance, *DL Contract* can be applied before and after model compilation or at any training stage. Here, we propose an effective algorithm to enforce runtime assertion capturing those properties.

Contextualized Inter-API Call Contracts: *DL Contract* needs to support *ML variable* involving multiple APIs at different stages of the ML pipeline. Conventionally, a contract

for an API specifies constraints on the formal parameters of that API method which does not look beyond the scope of that method. *DL Contract* needs to constrain formal parameters across multiple API calls (e.g., at lines 19-20 in Fig. 1).

Post-training Contracts: *DL Contract* needs to support properties afterward training to capture the training behavior of DNNs at different stages of the ML pipeline. As in DL applications, it is often necessary to put constraints on post-training constructs. To solve this issue, we specify desired training behavior with postconditions to prevent training bugs using *DL Contract* for respective training-related APIs.

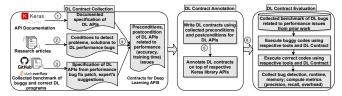


Figure 2. Methodology to collect and evaluate *DL Contract*.

4 Evaluation Methodology

In order to evaluate the *DL Contract*, we plan to collect deep learning contracts (in Fig. 2). In 1, we can use official Keras library documentation [3]. In particular, we consider the selection criterion from DL bugs from prior works [18, 20-23]. In (2), we plan to collect a list of state-of-the-art research articles [12–14]. In (3), we intend to collect contracts from state-of-the-art approaches that provide benchmarks of buggy and correct DL programs [20-23]. We plan to use these benchmarks to gather DL programs with better performance (e.g., accuracy, runtime). These benchmarks help to extract performance-related contracts from fix patches and expert-defined solutions. Lastly, in 4, we plan to combine all extracted contracts from all sources into a curated list, which targets DL program performance. To implement DL Contract, we propose to extend an open-source package PyContracts [11] and address discussed challenges (§3).

We plan to demonstrate the effectiveness of *ML variable* to provide an abstraction of the model architecture and training behavior. To show *DL Contract*'s applicability for real-world programs with performance bugs, in 5 we intend to write those contracts and annotate them on respective *Keras* APIs. After that, in 6 we plan to conduct experiments using the benchmarks and reported the results and analysis in terms of accuracy. We also plan to compare and contrast it against existing tools based on precision and recall performance metrics. Finally, we intend to compute the runtime and memory overhead of our proposed *DL Contract*.

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