Monadic Deep Learning

Performing monadic automatic differentiation in parallel

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The Java and Scala community has built a very successful big data ecosystem. However, most of neural networks running on it are modeled in dynamically typed programming languages. These dynamically typed deep learning frameworks treat neural networks as differentiable expressions that contain many trainable variables, and perform automatic differentiation on those expressions when training them.

Until 2019, none of the learning frameworks in statically typed languages provided the expressive power of traditional frameworks. Their users are not able to use custom algorithms unless creating plenty of boilerplate code for hard-coded back-propagation.

We solved this problem in DeepLearning.scala 2. Our contributions are:

- We discovered a novel approach to perform automatic differentiation in reverse mode for statically typed functions that contain multiple trainable variables, and can interoperate freely with the metalanguage.
- We designed a set of monads and monad transformers, which allow users to create monadic expressions that represent dynamic neural networks.
- Along with these monads, we provide some applicative functors, to perform multiple calculations in parallel.

With these features, users of DeepLearning.scala were able to create complex neural networks in an intuitive and concise way, and still maintain type safety.

Additional Key Words and Phrases: type class, path-dependent type, monad, scala

1 BACKGROUND AND INTRODUCTION

Deep neural networks have become the state of the art on many tasks, such as computer vision, game playing, voice recognition and natural language translation.

A neural network is a computation model that transforms the input, into output, by repeated application of tensor operations (including matrix multiplication, tensor resizing, element-wise operations, such as max, +, etc). A "deep" neural network just indicates there are large amount of such transformations.

Additionally, a neural network has additional hidden inputs, called parameters or weights, and deep learning is the task of finding the best weights for a neural network, such that a predefined objective (called loss) is minimized.

Deep learning is mostly done using different variation of gradient descend: we calculate the first order derivative of the loss function with respect to the weight, and update the weight accordingly. The processed is called backpropagation.

Thus, backpropagation[Rumelhart et al. 1985] is the key feature in many deep learning frameworks. Combined with other optimization algorithms[Duchi et al. 2011; Kingma and Ba 2014; Zeiler 2012], deep learning frameworks mutate the values of weights in neural networks during training, producing a model of knowledge learnt from training data.

Backpropagation can be considered as a specialized instance of Automatic Differentiation (AD)[Baydin et al. 2015b]. Many successful Python deep learning frameworks[Google Brain 2017; Neubig et al. 2017; Paszke et al. 2017; Tokui et al. 2015] implement a common set of features of auto differentiation:

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Reverse mode These deep learning frameworks perform reverse mode AD instead of forward mode, as forward mode AD does not scale well for deep neural networks.

Multiple trainable variable Neural networks are composed of multiple layers. Each layer contains their own trainable variables. These deep learning frameworks are able to calculate the derivatives of all trainable variables at once for one training data batch.

Internal DSL[Fowler 2010] These deep learning frameworks are libraries that provide an Internal DSL, allowing users to create their differentiable functions in Python or Lua from similar expressions as creating ordinary non-differentiable functions. Since these frameworks do not require external language, models created by them can be easily integrated into a larger application simply with higher-level configurations[Chollet et al. 2015] or ETL (Extract, Transform and Load) process.

However, how to archive those goals in statically typed library is still an open question. Previous solutions in statically type languages usually requires metaprogramming or compiler-time translation. In this paper, we present DeepLearning.scala, which is the first statically typed implementation that achieves all the above goals for deep neural networks. Our approach is based on some widely available functional programming constructs, thus can be ported to other statically typed programming languages.

2 BASIC CONCEPTS

For example, suppose we are building a robot for answering questions in IQ test like this:

> What is the next number in this sequence:
> 3, 6, 9, ?
> The answer is 12.

In DeepLearning.scala, the robot can be implemented as a `guessNextNumber` function as following[1]:

```
// Weight initialization
val weights: Seq[DoubleWeight] = Stream.continually(DoubleWeight(math.random))
val bias: DoubleWeight = DoubleWeight(math.random)

def guessNextNumber(question: Seq[Double]): DoubleLayer = {
  // Perform a dot product between question and weights
  (question zip weights).map {
    case (element, weight) => element * weight
  }.reduce(_ + _) + bias
}
```

Listing 1. The differentiable matrix multiplication implemented by `map`/`reduce`

`guessNextNumber` performs a dot product between question and weights by invoking higher-order functions `map` and `reduce`.

Unlike[Chen 2017]'s special tensor type, our tensor can be typed simply as `Seq[Double]`, `Seq[DoubleWeight]` or `Seq[DoubleLayer]`. [2]

[1]The code examples from Listing 1 to Listing 7 do not contain necessary **`import`** and configurations. For an executable model backed by ND4J[Skymind 2017b], see Getting Started documentation on DeepLearning.scala website.

[2]DeepLearning.scala users can use other representations of tensors: (1) For tensors with a statically typed shape, use `shapeless.Sized`. For example a 10×20 two-dimensional tensor can be typed as `Sized[Sized[Double, _10], _20]`.

The return value of `guessNextNumber`, along with temporary variables in `guessNextNumber`, are `DoubleLayers`, which are differentiable expressions.

The `weights` and `bias` contains some `DoubleWeight` that are referenced by `guessNextNumber`. They must be initialized before executing the model. Those are trainable variables.

From the user's point of view, both `DoubleLayer` and `DoubleWeight` are opaque types similar to an ordinary `scala.Double`. Most of the operators of `scala.Double` are also available on `DoubleLayer` and `DoubleWeight`, except those operators are differentiable. For now, the type signature of the multiplication operator as can be seen as in Listing 2, and we will reveal the real type signature of `*` in Section 4.

```
trait DoubleLayer {
  // Scalar multiplication
  def *(rhs: Double): DoubleLayer
  def *(rhs: DoubleLayer): DoubleLayer
  def *(rhs: DoubleWeight): DoubleLayer

  // Element-wise multiplication
  def *(rhs: INDArray): INDArrayLayer
  def *(rhs: INDArrayLayer): INDArrayLayer
  def *(rhs: INDArrayWeight): INDArrayLayer
}
trait DoubleWeight {
  // Scalar multiplication
  def *(rhs: Double): DoubleLayer
  def *(rhs: DoubleLayer): DoubleLayer
  def *(rhs: DoubleWeight): DoubleLayer

  // Element-wise multiplication
  def *(rhs: INDArray): INDArrayLayer
  def *(rhs: INDArrayLayer): INDArrayLayer
  def *(rhs: INDArrayWeight): INDArrayLayer
}
```

Listing 2. The hypothetical type signature of multiplication operator for `DoubleLayer` and `DoubleWeight`

Table 1 lists DeepLearning.scala built-in differentiable types other than `DoubleLayer` and `DoubleWeight`.

Table 1. Built-in Differentiable Types

	non-trainable value	trainable variable	differentiable expression
single-precision scalar	`Double`	`DoubleWeight`	`DoubleLayer`
double-precision scalar	`Float`	`FloatWeight`	`FloatLayer`
vector	`INDArray`	`INDArrayWeight`	`INDArrayLayer`

For differentiable tensors, replace vanilla `Double` to `DoubleWeight` or `DoubleLayer`. (2) For GPU-accelerated tensors, use `INDArray`[Skymind 2017b]. For differentiable tensors, use `INDArrayLayer` or `INDArrayWeight` instead.

In addition to differentiable operations, `Layers` and `Weights` can be evaluated with a `predict` method, thus, the model can predict the next Integer by calling an ordinary function, as shown in Listing 3. You may notice the `blockingAwait` suffix appended to `predict`, because `predict` returns a `Future[Double]` [3] , which contains the asynchronous task to compute the result. The actual computation is not performed in `predict` until `blockingAwait` is invoked[4].

```
val question = Seq(42.0, 43.0, 44.0)
println(guessNextNumber(question).predict.blockingAwait)
```

Listing 3. Inference on an untrained model

However, `guessNextNumber` returns an incorrect result because the weights and bias were randomly initialized, and have not been trained.

In order to train them, a loss function is necessary:

```
def squareLoss(robotAnswer: DoubleLayer, expectedAnswer: Double): DoubleLayer =
    {
  val difference: DoubleLayer = robotAnswer - expectedAnswer
  difference * difference
}
```

Listing 4. The differentiable square loss function

The above loss function `squareLoss` determines the squared error between robot's answer and the correct answer.

Both `squareLoss` and `guessNextNumber` are ordinary functions, and can be composed in other functions:

```
def linearRegression(question: Seq[Double], expectedAnswer: Double):
    DoubleLayer = {
  val robotAnswer = guessNextNumber(question)
  squareLoss(robotAnswer, expectedAnswer)
}
```

Listing 5. A differentiable function to train a linear regression model

`linearRegression`, composed of `guessNextNumber` and `squaredLoss`, returns a `DoubleLayer` of the loss for a specific question and its expected answer. `linearRegression` is a linear regression

[3] For readers familiar to Haskell, you can understand `Future` from the corresponding types in Haskell:

- `Future` is an opaque type alias of a `TryT`-transformed `UnitContinuation`, which is used for asynchronous operations with the ability of exception handling.
- "opaque type alias" is similar to the `newtype` feature in Haskell.
- `TryT` provides the ability of exception handling, which is similar to `ExceptT` monad transformer in Haskell.
- `UnitContinuation` is similar to `Cont ()` in Haskell, which is used for asynchronous operations, like an asynchronous version of `IO` in Haskell.

All the above types are general purpose libraries, not parts of DeepLearning.scala. We use those continuation based monadic data types to archive the ability of parallel and asynchronous execution.

[4] When `predict` is used in a real world scenario (e.g. running a neural network in a web service), `blockingAwait` should be replaced to `flatMap`, instead of blocking the current thread, which is an expensive resource. We use this `blockingAwait` here because it's more straightforward for understanding.

model with a square loss, and it can be trained as shown Listing 6. The `blockingAwait` is invoked because `train` returns a `Future[Double]` as well.

```
val question1 = Seq(3.0, 4.0, 5.0)
val expectedAnswer1 = 6.0

val question2 = Seq(13.0, 19.0, 25.0)
val expectedAnswer2 = 31.0

for (iteration <- 0 until 500) {
  linearRegression(question1, expectedAnswer1).train.blockingAwait
  linearRegression(question2, expectedAnswer2).train.blockingAwait
}
```

Listing 6. Training for 500 iterations

The weights and bias referenced by `linearRegression` are modified during 500 iterations of training, by stochastic gradient descent, to minimize the loss returned from `linearRegression`.

When weights and bias have been trained to make loss close to zero, `guessNextNumber` should return values that are very close to the expected answers.

```
val question = Seq(42.0, 43.0, 44.0)
println(guessNextNumber(question).predict.blockingAwait)
```

Listing 7. Inference on a trained model

This time, it will print a number clos to 45, as the model has finally learned the pattern of arithmetic progression.

The example from Listing 1 to Listing 7 demonstrated some basic concepts in DeepLearning.scala.

- `guessNextNumber`, `squareLoss` and `linearRegression` are differentiable functions that return differentiable expressions, which are computational graph nodes that can be evaluated when `train`ing or `predict`ing.
- Differentiable expressions and trainable variables can be used as if they are ordinary non-differentiable values. For example, as shown in Listing 4, you can perform scalar subtraction and multiplication between `DoubleWeight`, `DoubleLayer` and ordinary `scala.Double`.
- When `train`ing a differentiable expression, it returns a `Future`, which encapsulates the side-effect of adjusting trainable variables referenced by the differentiable function.
- If a differentiable function invokes another differentiable function, then trainable variables trained by one differentiable function affect another one. For example, when training the differentiable function `linearRegression`, The trainable variables `weights` and `bias` are modified, hence `guessNextNumber` automatically gains the ability to `predict` correct answers.

3 DYNAMIC NEURAL NETWORKS

DeepLearning.scala supports dynamic neural networks. It means that the control flow of a neural network can differ according to values of internal nodes of the computational graph, when processing a specific batch of input. This is the key feature of recent deep learning frameworks

like PyTorch[Paszke et al. 2017] or Chainer[Tokui et al. 2015]. Especially, dynamic deep neural networks can be more efficient by skipping part of the model[Liu and Deng 2017].

In this section, we will present how to create a simple dynamic neural network in DeepLearning.scala, which can be considered as a simplified version of outrageously large neural networks[Shazeer et al. 2017].

Suppose we have two sub-neural networks, `leftSubnet` and `rightSubnet` (Listing 8)[5]. We want to build a "gated" network, which conditionally runs either `leftSubnet` or `rightSubnet` for a special `input`.

```
def leftSubnet(input: INDArrayLayer): INDArrayLayer
def rightSubnet(input: INDArrayLayer): INDArrayLayer
```

Listing 8. Predefined sub-networks

Which sub-network is selected for the `input` should be determined by the `gate` network, which returns a pair of differentiable double expressions that indicate the preferences between `leftSubnet` and `rightSubnet`, shown in (Listing 9).

```
def gate(input: INDArrayLayer): (DoubleLayer, DoubleLayer)
```

Listing 9. Predefined gate network

The differentiable operations on `DoubleLayers` and `INDArrayLayers` form a differentiable embedded DSL inside the meta-language Scala. Thus, the concept of "gated" neural network can be considered as a conditional control flow in the differentiable DSL, and the values of nodes of a gated neural network are simply some let bindings in the DSL.

The control flow of the gated network that we want to build is described in Function GatedNetwork.

Function GatedNetwork

Input: Features extracted by preceding layers
Output: Features passed to succeeding layers
scores ← `gate`(*Input*);
if *score of left sub-network* > *score of right sub-network* **then**
  return *score of left sub-network* × `leftSubnet`(*Input*);
else
  return *score of right sub-network* × `rightSubnet`(*Input*);
end

In DeepLearning.scala, there are three different approaches to implement the gated network. Examples of these approaches are introduced in following Section 3.1, Section 3.2, and Section 3.3.

3.1 Eager Execution (bad)

An obvious approach to create the gated network is to eagerly execute the `gate`, shown in Listing 10:

There are three sub-networks in the `naiveGatedNet` function. The `gate` returns a pair of `DoubleLayers`. By blocking await the `prediction` result, we get two `Doubles`, which can be used

[5] For performance purpose, instead of `Seq[DoubleLayer]`, we use `INDArrayLayer` as the type of differentiable expression backed by ND4J. `INDArrayLayer` supports differentiable version of most operations that ND4J's n-dimensional array `INDArray` supports.

```
def naiveGatedNet(input: INDArrayLayer): INDArrayLayer = {
  val scores = gate(input)
  if (scores._1.predict.blockingAwait > scores._2.predict.blockingAwait) {
    scores._1 * leftSubnet(input)
  } else {
    scores._2 * rightSubnet(input)
  }
}
```

Listing 10. The eager execution implementation of gated network

to determine which sub-network is preferred between `leftSubnet` and `rightSubnet`. The chosen sub-network will be multiplied with the value returned by the `gate` in order to enabling backpropagation on the `gate`.

However, there is a performance issue in the `naiveGatedNet`.

In DeepLearning.scala, all differentiable expressions, including the scalar `DoubleLayer` and vectorized `INDArrayLayer`, contain some lazily evaluated differentiable computational graph nodes, which will not be executed until a `predict` or `train` task is performed in a `blockingAwait` or `onComplete` call.

So, the two `predict.blockingAwait` calls in the **`if`** will execute the computational graph in `gate` twice. Also the computational graph in `naiveGatedNet` will be executed when users call `predict` or `train` in the future. Even worse, `input` contains a computational graph, too. Along with `gate`, it will be evaluated three times, which may contain a complex future extracting process.

3.2 Monadic Control Flow (good)

Ideally, the calls to `predict` should be avoided in differentiable functions. The recommended approach to create a dynamic neural network is using `forward`, which returns a monadic value of `Do[Tape[Data, Delta]]`, which can be used in a monadic control flow via Scalaz[Yoshida 2017]'s type classes[Oliveira et al. 2010] `Monad` and `Applicative`.

Listing 11 shows the monadic control flow of a gated network. The gated network is built from the monadic expression `gatedForward`, which contains some `forward` calls, which are asynchronous operations (or `Do`) that produce Wengert list records (or `Tape`s). The implementation details of `Do` and `Tape` will be discussed in Section 5. For now, we only need to know that `Do` is a monadic data type that supports `flatMap`.

By `flatMap`ping those `forward` operations together, we built the entire monadic control flow `gatedForward` for the gated network.

The `monadicGatedNet` represents a dynamic neural network, since each `forward` operation is started after its previous `forward` is done. This behavior allows for dynamically determining succeeding operations according to results of previous `forward` operations, as shown in the **`if`** clause in Listing 11.

However, `flatMap` prevents additional optimization, too. `scores._2.forward` have to wait for `scores._1.forward`'s result, even if the two operations are logically independent.

3.3 Parallel Applicative Control Flow + Sequential Monadic Control Flow (better)

Ideally, the independent operations `scores._1.forward` and `scores._2.forward` should run in parallel. This can be done by tagging `Do` as `Parallel`, and use `scalaz.Applicative.tuple2` [McBride and Paterson 2008] instead of `flatMap` (Listing 12).

```
def monadicGatedNet(input: INDArrayLayer): INDArrayLayer = {
  val scores = gate(input)
  val gatedForward: Do[Tape[INDArray, INDArray]] = {
    scores._1.forward.flatMap { tape1: Tape[Double, Double] =>
      scores._2.forward.flatMap { tape2: Tape[Double, Double] =>
        if (tape1.data > tape2.data) {
          (scores._1 * leftSubnet(input)).forward
        } else {
          (scores._2 * rightSubnet(input)).forward
        }
      }
    }
  }
  INDArrayLayer(gatedForward)
}
```

Listing 11. Monadic gated network

```
def applicativeMonadicGatedNet(input: INDArrayLayer): INDArrayLayer = {
  val scores = gate(input)
  val parallelForward1: ParallelDo[Tape[Double, Double]] = {
    Parallel(scores._1.forward)
  }
  val parallelForward2: ParallelDo[Tape[Double, Double]] = {
    Parallel(scores._2.forward)
  }
  val Parallel(stage1) = {
    parallelForward1.tuple2(parallelForward2)
  }
  def stage2(tapes: (Tape[Double, Double], Tape[Double, Double])) = {
    if (tapes._1.data > tapes._2.data) {
      (scores._1 * leftSubnet(input)).forward
    } else {
      (scores._2 * rightSubnet(input)).forward
    }
  }

  val gatedForward = stage1.flatMap(stage2)
  INDArrayLayer(gatedForward)
}
```

Listing 12. Applicative + monadic gated network

This `applicativeMonadicGatedNet` takes both advantages from applicative functors and monads. The entire control flow is a `flatMap` sequentially composed of two stages. In `stage1`, there is a `tuple2` composed of `scores._1.forward` and `scores._2.forward` in parallel. Then, in `stage2`, the succeeding operation is dynamically determined according to `tapes`, the result of `stage1`.

The parallel applicative operation is also the default behavior for all built-in vector binary operators. Listing 13 shows some simple expressions that will be executed in parallel.

```
def parallelByDefault(a: INDArrayLayer, b: INDArrayLayer, c: INDArrayLayer, d:
    INDArrayLayer): INDArrayLayer = {
  a * b + c * d
}
```

Listing 13. By default, `a * b` and `c * d` will be executed in parallel because they are independent

By combining both applicative functors and monads, DeepLearning.scala supports dynamic neural network and still allows the independent parts of the neural network to run in parallel. In addition, the backward pass of differentiable functions built from parallel applicative functors or built-in vector binary operators will be executed in parallel, too.

3.4 Direct style DSL for Applicative and Monadic Control Flow (best)

In the previous section, we had presented a dynamic neural network executed in parallel. However, the usage of `flatMap` and `Parallel`-tagged types may scare algorithm authors who are not familiar with monadic programming. Ideally, the code written by those people should look straightforward and has the same structure in pseudo-code GatedNetwork or Listing 10, and still gain the benefits of Listing 12.

The goal can be achieved by transforming the direct style code into monadic and applicative code at compile-time. We created an DSL with the help of the !-notation provided by Dsl.scala[Yang 2017], which provides Scala compiler plugins to perform the necessary compiler-time transformation.

As shown in Listing 14, the !-notation "extracts" the `Double` values from a pair of `DoubleLayers` in parallel. Those `Doubles` are ordinary non-differentiable Scala types that will not backpropagate, and can be used in ordinary Scala control flow expression like **`if`**.

```
def dslGatedNet(input: INDArrayLayer): INDArrayLayer = {
  val scoreLayers: (DoubleLayer, DoubleLayer) = gate(input)
  val scores: (Double, Double) = !scoreLayers
  if (scores._1 > scores._2) {
    scoreLayers._1 * leftSubnet(input)
  } else {
    scoreLayers._2 * rightSubnet(input)
  }
}
```

Listing 14. Dsl.scala powered direct style gated network

Generally, a !-notation on a `Layer` will generate a monadic `flatMap` call, to extract the value of forward pass of the `Layer`; a !-notation on a tuple of `Layers` will generate some applicative `<*>` and `map` calls, to extract a tuple of values of forward pass of those `Layers`, in parallel. Thus, the actually code generated by Dsl.scala's compiler plugins for Listing 14 is similar to Listing 12.

4 AD HOC POLYMORPHIC DIFFERENTIABLE FUNCTIONS

In section 2, we had presented the hypothetical differentiable types of multiplication for `DoubleLayer` and `DoubleWeight`. However, the method overloading approach shown in Listing 2 is too verbose,

and requires a lot of boilerplate code. In this section, we will present an approach to create custom differentiable functions, without such methods overloading.

A differentiable function is a neural network. Ideally, a differentiable function should be an ad hoc polymorphic function that accepts heterogeneous types of parameters, including:

- A vanilla vector input. i.e. `INDArray`.
- Differentiable expressions of hidden states produced by any previous neural network layers, i.e. any `INDArrayLayers` regardless of the prefixes.
- Trainable variables in the case of activation maximization technique[Erhan et al. 2009].i.e. any `INDArrayWeights` regardless of the prefixes.
- Other user defined differentiable type.

Table 1 shows nine types that have built-in `DeepLearning` type classes.

This can be achieved with the help of[Gurnell 2017]'s Scala encoding of dependent-type type class. We defined a `DeepLearning` (Listing 15[6]) type class that witnesses any supported expressions including differentiable expressions, trainable variables, or vanilla non-differentiable types. The users can create type aliases to restrict the types of state during forward pass and backward pass as shown in Listing 16.

```
trait DeepLearning[Differentiable] {
  /** The type of result calculated during forward pass */
  type Data

  /** The type of derivative during backward pass */
  type Delta

  def forward(differentiable: Differentiable): Do[Tape[Data, Delta]]
  // Other auxiliary methods is omitted
}
```

Listing 15. The dependent-type type `DeepLearning`

```
type INDArrayExpression[Expression] = DeepLearning[Expression] {
  /** The type of result calculated during forward pass */
  type Data = INDArray

  /** The type of derivative during backward pass */
  type Delta = INDArray
}
```

Listing 16. A type class alias that witnesses dense vector expressions

By using `INDArrayExpression` as a context bound, we can create a polymorphic differentiable function that accepts any vector expression.

[6] For readers who are more familiar with Idris, there is a corresponding notation in Idris:

```
interface DeepLearning Differentiable where
  Data : Type
  Delta : Type
  forward : Differentiable -> Do (Tape Data Delta)
```

```
def polymorphicDifferentiableFunction[A: INDArrayExpression, B:
    INDArrayExpression, C: INDArrayExpression, D: INDArrayExpression](a: A, b:
    B, c: C, d: D): INDArrayLayer = {
  a * b + c * d
}
```

Listing 17. A polymorphic differentiable function

Listing 17 is similar to Listing 13, except each argument of `polymorphicDifferentiableFunction` accepts `INDArray`, `INDArrayWeight` or `INDArrayLayer` respectively, not only `INDArrayLayer`.

Built-in operations including arithmetic operations, `max`, and `dot` are polymorphic differentiable functions defined in this approach, too, which can be used in user-defined polymorphic differentiable functions.

5 IMPLEMENTATION

In this section, we will introduce the internal data structure used in DeepLearning.scala to perform AD.

- For ease of understanding, Section 5.1 starts from a simple dual number implementation `DualNumber`, which was known as an approach to perform forward mode AD for scalar values.
- Section 5.2 introduces our variation of dual number `ClosureBasedDualNumber`, which supports tree-structured reverse mode AD (aka backpropagation) for multiple trainable variables.
- Section 5.3 shows the actual data type `Tape` in DeepLearning.scala, which is generalized to not only scalar types, but also vector types and any other differentiable types.
- Section 5.4 discovers the monadic control flow `Do`, which manages the life cycle of `Tape`s, sharing `Tape`s for common computational graph nodes, allowing for an arbitrary DAG(Directed Acyclic Graph)-structured computational graph.
- Section 5.5 summarizes the entire execution process during a training iteration, showing how the user-defined differentiable functions get executed through internal mechanisms `Do` and `Tape`.

5.1 Ordinary Dual Number

Our approach for reverse mode AD uses a data structure similar to traditional forward mode AD, with only a few changes.

Forward mode AD can be considered as computation on dual number. For example, dual number for scalar types can be implemented as Listing 18:

```
type Data = Double
type PartialDelta = Double
case class DualNumber(data: Data, delta: PartialDelta)
```

Listing 18. Dual number for forward mode AD

Arithmetic operations on those dual number can be implemented as Listing 19:

5.2 Monadic Closure-based Dual Number

However, it is hard to type this approach if we want to support multiple trainable variables, with the number unknown before runtime. `PartialDelta` in Listing 18 represents the partial derivative

```
object DualNumber {
  def plus(left: DualNumber, right: DualNumber): DualNumber = {
    DualNumber(left.data + right.data, left.delta + right.delta)
  }
  def multiply(left: DualNumber, right: DualNumber): DualNumber = {
    DualNumber(left.data * right.data, left.data * right.delta + right.data *
        left.delta)
  }
}
```

Listing 19. Arithmetic operations on dual number

of trainable variables. In AD tools that support only one trainable variable, the trainable variable is usually forced to be the input. Hence `PartialDelta` is the input type for those AD tools. This assumption is broken for our case, since our delta type of a specific `DualNumber` must contain derivatives for all trainable variables that were used to produce the `DualNumber`, not only the partial derivative of input. As a result, the type of delta varies when the number of trainable variables grows.

To type-check the delta, considering the only usage of the delta in a neural network is in updating trainable variables in a gradient descent based optimization algorithm, we can replace `PartialDelta` to an `UpdateWeights` closure as shown in Listing 20.

```
type Data = Double
case class ClosureBasedDualNumber(data: Data, backward: UpdateWeights)
```

Listing 20. Replacing `PartialDelta` to a closure

Unlike `PartialDelta`, `UpdateWeights` is not a number that supports native arithmetic operations, thus we have to replace native arithmetic operations on `PartialDelta` to some static functions on `UpdateWeights` when implement arithmetic operations for the new dual number, as shown in Listing 21

The only question remaining is to implement the `UpdateWeights`, to make its behavior be equivalent to the original dual number implementation.

Mathematically, the `UpdateWeights` type in a dual number should form any vector space, i.e. the `UpdateWeights` closure itself must support addition and scalar multiplication operations.

Our approach is making `UpdateWeights` be a function type that contains side-effects to update trainable variables. Thus the addition operation for closures can be defined as (1).

$$(f_0 + f_1)(x) = f_0(x) + f_1(x) \tag{1}$$

And the scalar multiplication operation for closures is defined as (2):

$$(x_0 f)(x_1) = f(x_0 x_1) \tag{2}$$

The above definition of arithmetic operations can be implemented in monadic data types as shown in Listing 22.

`UpdateWeights`, as a replacement to original `PartialDelta`, is a closure able to update derivatives for all weights with a coefficient (the `Double` parameter). `|+|` is the append operation of `Semigroup`, which could be any cumulative data type.

```
object ClosureBasedDualNumber {
  def plus(left: ClosureBasedDualNumber, right: ClosureBasedDualNumber):
      ClosureBasedDualNumber = {
    ClosureBasedDualNumber(left.data + right.data, UpdateWeights.plus(left.
        backward(), right.backward()))
  }
  def multiply(left: ClosureBasedDualNumber, right: ClosureBasedDualNumber):
      ClosureBasedDualNumber = {
    ClosureBasedDualNumber(
      left.data * right.data,
      UpdateWeights.multiply(left.data, right.backward()) + UpdateWeights.
          multiply(right.data, left.backward()))
  }
}
```

Listing 21. Replacing operations on `PartialDelta` to custom functions for `UpdateWeights`

```
type UpdateWeights = Do[Double] => SideEffects
object UpdateWeights {
  /** (f0 + f1)(x) = f0(x) + f1(x) */
  def plus(f0: UpdateWeights, f1: UpdateWeights) = { doX: Do[Double] =>
    f0(doX) |+| f1(doX)
  }

  /** (x0 f)(x1) = f(x0 x1) */
  def multiply(x0: Double, f: UpdateWeights) = { doX1: Do[Double] =>
    f(doX1.map(x0 * _))
  }
}
```

Listing 22. Arithmetic operations for the closure that contains side-effects

Also note that the parameter is a monadic data type `Do` that encapsulates the computation of derivative. Unlike strictly evaluated values, `Do` is an operation only evaluated when needed.

In DeepLearning.scala, our `SideEffects` is based on the asynchronous operation type `UnitContinuation`. Our built-in differentiable operations execute the independent parts of backward pass in parallel with the help of `Applicative` type class instances of `UnitContinuation`.

```
type SideEffects = UnitContinuation[Unit]
```

Listing 23. Monadic side-effects

`UnitContinuation[A]` is an opaque alias[Osheim and Cantero 2017] of `(A => Trampoline[Unit]) => Trampoline[Unit]`, implemented in a separate library at future.scala. It is used in DeepLearning.scala as a monadic data type for encapsulating side effects in stack-safe asynchronous programming.

The SideEffects for neural networks conform to the associative law because the only side effects is updating trainable variables. Thus, our UpdateWeights.plus and UpdateWeights.multiply are equivalent to the operations on strictly evaluated scalar value PartialDelta in forward mode AD.

Since UpdateWeights is a closure with side effects, a trainable variable can be represented as a tuple of a mutable value and the action to modify the mutable value.

```
def createTrainableVariable(initialValue: Double, learningRate: Double):
    ClosureBasedDualNumber = {
  var data = initialValue
  val backward: UpdateWeights = { doDelta: Do[Double] =>
    val sideEffects: Do[Unit] = doDelta.map { delta =>
      data -= learningRate * delta
    }
    convertDoToContinuation(sideEffects)
  }
  ClosureBasedDualNumber(data, backward)
}
```

Listing 24. Create a dual number for a trainable variable

In Listing 24, the trainable variable is trained by a fixed learning rate to simplify the hyperparameters of optimization algorithms. The sideEffects is the only code in the entire code base that performs native side effects. The actual DeepLearning.scala implementation has a more sophisticated mechanism to customize the implementation of side effects, allowing other optimizers and custom hyperparameters.

Similar to trainable variables, a non-trainable value can be represented as a tuple of the value and a no-op closure as shown in Listing 25.

```
def createLiteral(data: Double): ClosureBasedDualNumber = {
  val backward = { doDelta: Do[Double] =>
    UnitContinuation.now(())
  }
  ClosureBasedDualNumber(data, backward)
}
```

Listing 25. Create a dual number for a non-trainable value

Because delta is an action instead of pre-evaluated value, the implementation of backward for a non-trainable value can entirely avoid executing any unnecessary computation in doDelta.

Finally, we can create a differentiable function as shown in Listing 26, whose leaf nodes are createTrainableVariable and createLiteral, and internal nodes are arithmetic operations in Listing 21.

The computational graph of computationalTree is shown in Figure 1. Note that the arrow direction denotes the dependency between expressions, from arrow tail to arrow head, which is the reverse of the direction of data flow.

The closure-based dual number y1 has a closure backward, which returns SideEffects that recursively change all trainable variables referenced by the closure.

```
val w0 = createTrainableVariable(math.random, 0.001)
val w1 = createTrainableVariable(math.random, 0.001)

def computationalTree(x: ClosureBasedDualNumber) = {
  val y0 = ClosureBasedDualNumber.multiply(x, w0)
  val y1 = ClosureBasedDualNumber.multiply(y0, w1)
  y1
}
```

Listing 26. A tree-structured differentiable function

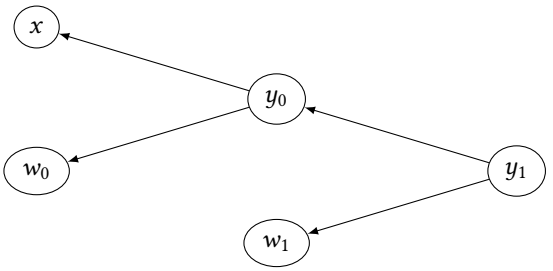

Fig. 1. A tree-structured computational graph

Note that backward itself does not perform any side effects. It just collects all side effects into a `UnitContinuation[Unit]`. Figure 2 shows how the side effects of updating trainable variables are collected.

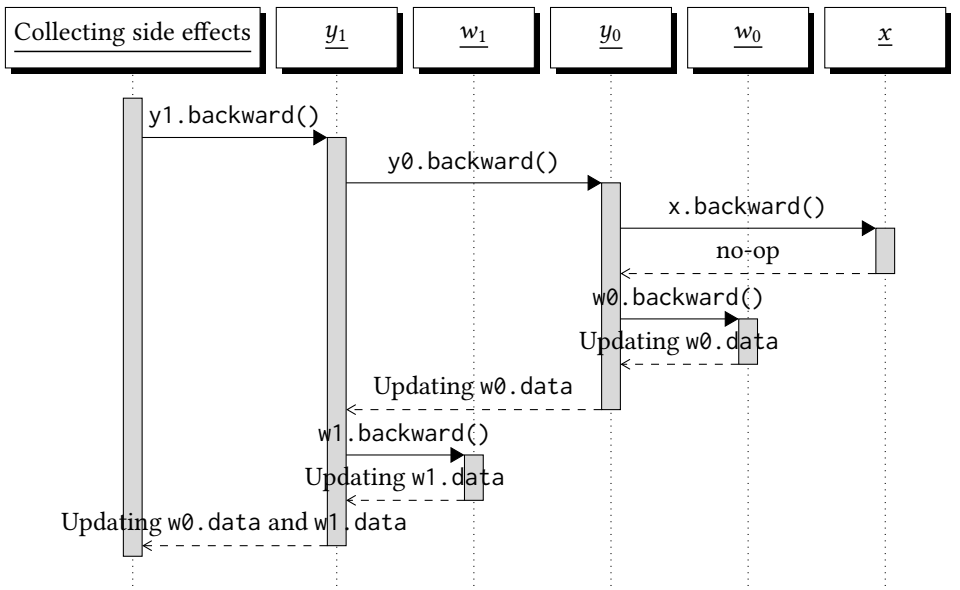

Fig. 2. Backpropagation for a tree-structured computational graph

Finally, the collected side effects of `UnitContinuation[Unit]` returned from `y1.backward` can be performed by a `blockingAwait` or `onComplete` call.

5.3 Generic Tape

This closured-based monadic dual number can be generalized to any linear spaces, not only scalar types such as `Double`, but also n-dimensional arrays.

The dual number type that we actually defined in DeepLearning.scala is `Tape`, a generic version of `ClosureBasedDualNumber` in Listing 20. We replaced `ClosureBasedDualNumber`'s hard-coded `Double` to type parameters `Data` and `Delta`, as shown in Listing 27.

```
final case class Tape[+Data, -Delta](
  data: Data,
  backward: Do[Delta] => UnitContinuation[Unit]
)
```

Listing 27. Generic closured-based monadic dual number

`Data` and `Delta` are usually the same, but they can also be different types. For example, you can create a type whose `Data` is a dense n-dimensional array and whose Delta is a pair of index and scalar, representing a dense tensor that sparsely updates.

This data structure is similar to a Wengert list in traditional reverse mode AD, except our tape is a tree of closures instead of a list.

5.4 Reference Counted Tape

Although the closured-based dual number approach from Listing 20 to Listing 27 supports multiple trainable variables, the closure-based computation has a performance issue in the case of diamond dependencies.

Listing 28 shows a differentiable function `diamondDependentComputationalGraph` that contains diamond dependencies to some differentiable expressions or trainable variables.

```
val w = createTrainableVariable(math.random, 0.001)
def diamondDependentComputationalGraph(x: ClosureBasedDualNumber) = {
  val y0 = ClosureBasedDualNumber.multiply(x, w)
  val y1 = ClosureBasedDualNumber.multiply(y0, y0)1
  val y2 = ClosureBasedDualNumber.multiply(y1, y1)
  y2
}
```

Listing 28. A diamond dependent differentiable function

The computational graph of `diamondDependentComputationalGraph` are shown in Figure 3.

When `y2.backward` is invoked, in order to collect side effects of `y2`'s dependencies, `y1.backward` will be invoked, twice, and each `y1.backward` call will triggers two `y0.backward` calls. As a result, for each iteration of backpropagation, `y0.backward`, `w.backward` and `x.backward` are invoked four times, respectively.

The process in `y2.backward` is shown in Figure 4.

Generally, given n levels of nested diamond dependencies, the computational complexity is $O(2^n)$, which is unacceptable for neural networks that may share common differentiable expressions.

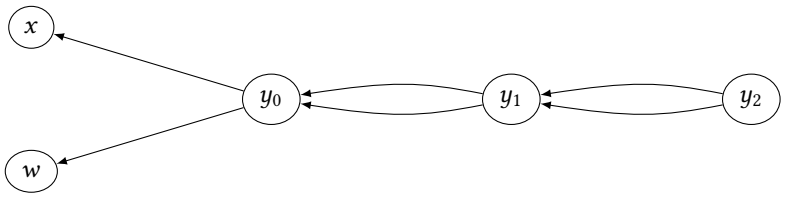

Fig. 3. A diamond dependent computational graph

We introduced a reference counting algorithm for dual numbers, to avoid the exponential time complexity, by only calling backward once.

The reference counting is managed in a wrapper of `Tape`, which has additional `acquire` and `release` functions.

Each wrapper has two internal states: (1) reference counter, (2) accumulator of delta. Respectively, `acquire` and `release` calls will increase and decrease the reference counter, and `backward` calls will cumulate the `delta` to the accumulator.

When the reference counting algorithm is enabled, `backward` is not recursive any more. Instead, a wrapper only call `backward` of its dependencies when the reference counter is decreased to zero. The entire process of backpropagation is shown in Figure 5.

This wrapper is implemented as the monadic data type `Do`, in which the side effects of updating counters and accumulators are monadic control flows. With the help of `Do`, now our computational graphs are modeled in `Do[Tape[Data, Delta]]`, which can be created by `forward` methods described in Section 3.2. As mentioned in Section 3.3, computational graph node of binary operations are evaluated in parallel.

In a traditional backpropagation implementation, tape is a list, hence both the execution order of backward pass and forward pass must be sequentially reverse to each other. Even a previous attempt of closure-based tape[Pearlmutter and Siskind 2008] still requires conversion to sequential expressions of A-normal form[Sabry and Felleisen 1993].

By introducing reference counting, the execution order of our backward pass and forward pass do not have to be exactly reverse, hence the conversion to A-normal form becomes unnecessary. As a result, DeepLearning.scala supports out-of-order execution in both forward pass and backward pass, in which the independent sub-graph can be even executed in parallel.

5.5 The Overview of a Training Iteration

In brief, in each iteration, a differentiable function that contains multiple trainable variables can be trained in the following steps:

(1) Executing the user-defined differentiable function with a batch of input, to obey a differentiable expression (i.e. a subtype of `Layer`).
(2) Calling `forward` on differentiable expression to build a computational graph (i.e. a `Do[Tape[Data, Delta]]`). The reference counter to the computational graph is zero at the point.
(3) Performing the `forward` pass of differentiable expression to build a tape (i.e. a `Tape[Data, Delta]`), which contains a pair of the result of forward pass and a `backward` closure. The reference counter of each node in a computational graph is increased during this step.
(4) Performing `backward` closure of the root node of the computational graph. The accumulator of delta on the root node is updated.

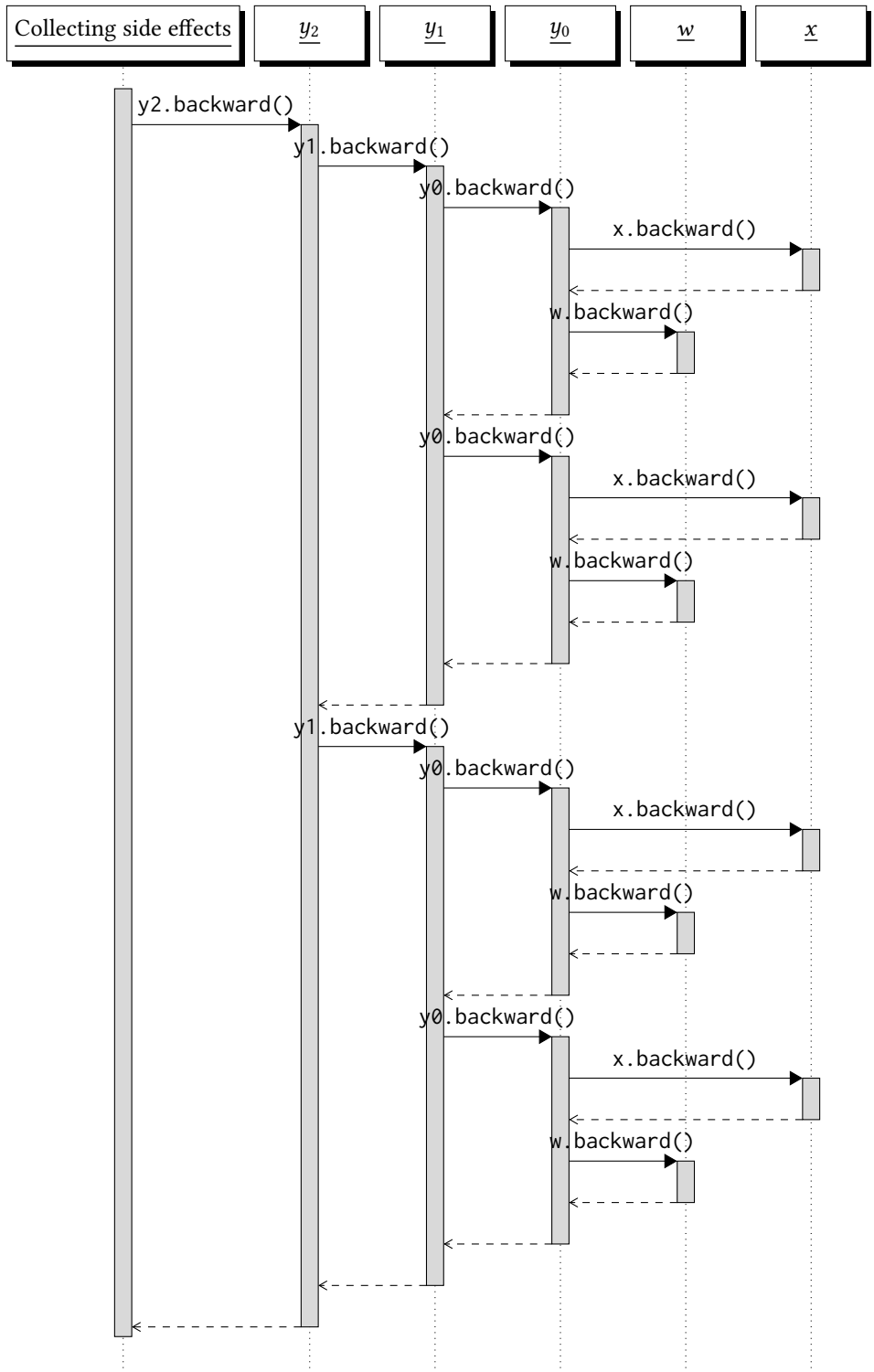

Fig. 4. Backpropagation for a diamond dependent computational graph

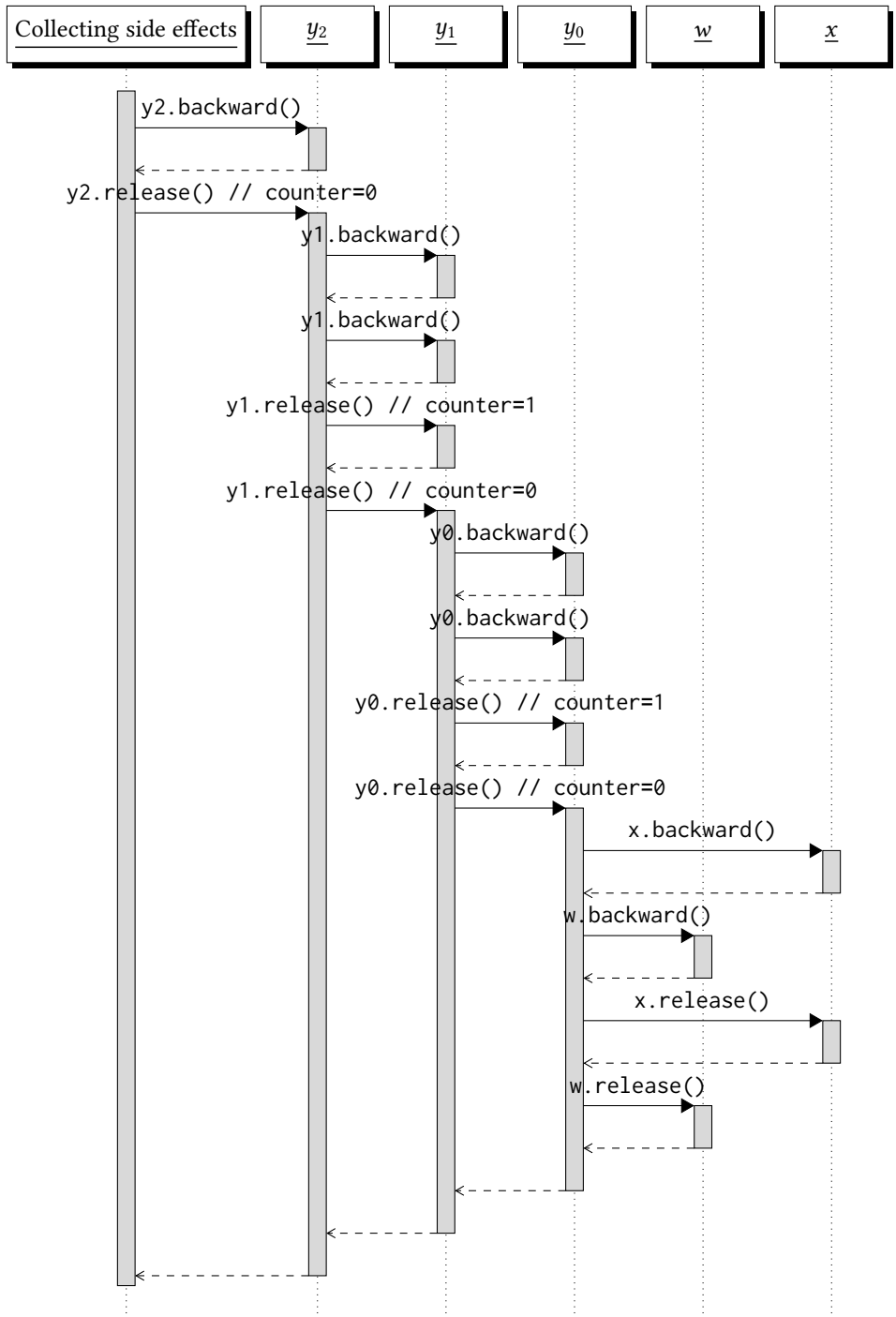

Fig. 5. Backpropagation for a diamond dependent computational graph (with reference counting)

(5) Releasing of the root node of the computational graph. The reference counter of each node in a computational graph is decreased to zero and the `backward` closure of each node is performed during this step, thus all referenced trainable variables are updated.

Note that step 1 and step 2 are pure function calls, with no side effects. Step 3 to step 5 are monadic control flows, which encapsulate some side effects that will be performed only when an unsafe method `blockingAwait` or `onComplete` is eventually called.

6 EVALUATION

We created some benchmarks to evaluate the computational performance of DeepLearning.scala, especially, we want to measure:

(1) How parallel execution affect the time cost of a training iteration of different structured neural networks;
(2) the computational performance impact when a part of a neural network is disabled.

Those benchmarks are built with Jmh[Shipilev 2018], running on CPU, measuring the number of mini-batches per second, for training neural networks that contain variant number of branches of sub-networks, as classifiers for CIFAR-100[Krizhevsky and Hinton 2009], which is a dataset for image recognition, which has 100 fine-grained classes containing 600 images each. These fine-grained classes are grouped into 20 coarse-grained classes.

The architecture of the network used for benchmarks summarized in Figure 6.

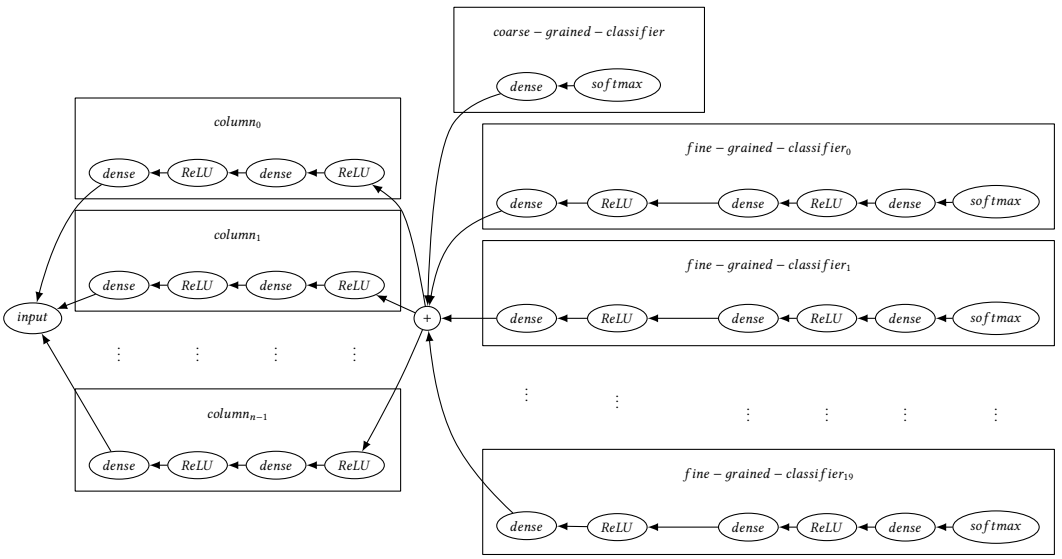

Fig. 6. The models used for benchmarks

We created *n* columns[Ciregan et al. 2012] of experts sub-networks for feature extracting. The output from those experts are then summed for further layers and classifiers. Each column contains two dense layers [7] followed by ReLU activation layers. Those columns are independent, and we expect our framework can execute them in parallel when training or inference.

[7] We use dense layers instead of convolution layers because the underlying N-dimensional array library ND4J is not able to efficiently perform immutable operation of convolution. See section 7.1 for discussion.

Since CIFAR-100 dataset has both coarse-grained and fine-grained labels, we created a coarse-grained classifier and 20 fine-grained classifiers. The coarse-grained classifier contains a dense layer to convert features to scores of 20 coarse-grained classes, followed by a softmax layer. Each fine-grained classifier corresponding to a coarse-grained class contains three dense layers, two ReLU activation layers, and a softmax layer, classifying 5 fine-grained classes.

We constructed mini-batches by a coarse-grained class when training. All samples in a mini-batch belongs to one coarse-grained class. With the help of the feature of dynamic neural network in DeepLearning.scala, for each training iteration, only one fine-grained classifier is used, other 19 fine-grained classifiers are skipped. When inferencing, the fine-grained classifier is chosen dynamically according to the prediction by the coarse-grained classifier. For comparison, we also created another set of benchmarks that do not skip unmatched fine-grained classifiers.

The benchmark result when training these models is shown in Table 2 and Table 3 (larger score is better). The sizes of those dense layers previous to softmax layers in these models are the number of classes (20 for coarse-grained classifier, 5 for fine-grained classifiers). Other dense layers output 64 features. These models are trained in a SGD optimizer with batch size 16. Both the number of columns in each model and the number of threads used in training vary among benchmarks.

number of columns	thread pool size	Score, ops/s	
4	1	2.550	± 0.043
4	2	3.233	± 0.276
4	4	3.338	± 0.217
2	1	3.345	± 0.095
2	2	3.987	± 0.091
2	4	4.828	± 0.200
1	1	3.854	± 0.046
1	2	5.239	± 0.288
1	4	6.328	± 0.058

Table 2. The benchmark result when no fine-grained classifier is skipped

number of columns	thread pool size	Score, ops/s	
4	1	5.314	± 0.304
4	2	5.484	± 0.362
4	4	5.607	± 0.159
2	1	8.702	± 0.430
2	2	9.527	± 0.259
2	4	8.831	± 0.268
1	1	12.430	± 1.514
1	2	13.531	± 0.618
1	4	14.513	± 0.554

Table 3. The benchmark result when unmatched fine-grained classifiers are skipped

The benchmark result verified the performance improvement when increasing thread pool size, since DeepLearning.scala executes independent sub-networks in parallel. This benchmark also shows a performance improvement when unmatched fine-grained classifiers are skipped.

7 FUTURE WORKS

7.1 New Back-end

Currently, DeepLearning.scala 2's built-in differentiable vector expression type `INDArrayLayer` is based on nd4j's `INDArray`[Skymind 2017b]. As described in Section 5.5, in each training iteration, for each computational graph node, `forward` and `backward` operations are performed, which internally call some methods on `INDArray`, resulting in GPU kernel executions for nd4j's CUDA runtime. These ND4J operations have bad computational performance because: (1) ND4J is not designed for immutable tensors;[8] (2) some operations[9] are extremely slow; (3) enqueuing a kernel is relatively expensive.

We are developing a new back-end as an alternative to nd4j. The new back-end will be able to merge multiple primitive operations into one larger kernel by dynamically generating OpenCL code. The new back-end will support more optimized operations on the GPU and reduce the number of kernel executions. We expect our new version will achieve better computational efficiency.

7.2 Distributed Model

Current DeepLearning.scala is only able to run on a standalone JVM, not a distributed cluster, thus it does not support "outrageously large neural networks"[Shazeer et al. 2017] that do not fit into the memory of a single node.

Since our computational graph is made of monadic expressions that consist of closures, they can be serialized and executed remotely in theory. We are investigating how to build a distributed machine learning system based on remotely executed monadic expression. We will find out if this suggested approach can support more complex models than the parameter server approach can.

8 DISCUSSION

DeepLearning.scala is an unique library among all deep learning frameworks. Our approach of AD has some attributes that never appear in previous frameworks.

8.1 Interoperable Differentiable Computational Graph

There were two different mechanisms in state-of-the-art deep learning frameworks: Define-and-Run vs. Define-by-Run.

State-of-the-art Define-and-Run frameworks[Abadi et al. 2016; Bergstra et al. 2010; Chen et al. 2015; Collobert et al. 2008; Intel 2016; Jia et al. 2014; Skymind 2017a] allows users to create computational graphs, which are immutable Abstract Syntax Trees (ASTs) of some object languages which can be evaluated by the framework runtime. Define-and-Run frameworks can schedule computational graphs to multiple CPUs, GPUs or other devices. However, the object languages have bad interoperability with the metalanguage. For example, a DeepLearning4j user cannot use Java control flows nor call Java native methods in neural networks.

State-of-the-art Define-by-Run frameworks[Google Brain 2017; Neubig et al. 2017; Paszke et al. 2017; Tokui et al. 2015] can eagerly execute actual forward pass calculation in user written code, and, at the same time, generate the internal states for running backward pass. Unlike Define-and-Run frameworks, Define-by-Run frameworks have good interoperability with the hosting language. Control flows and native function calls can be easily used during the execution of neural networks. However, Define-and-Run frameworks tend to store states and perform side effects when defining neural network structures, which makes this mechanism unsuitable for implementation in a purely functional flavor.

[8] https://github.com/deeplearning4j/nd4j/issues/2271#issuecomment-344865418
[9] `INDArray.broadcast` for example

We discovered the third mechanism of monadic deep learning. Neural networks in DeepLearning.scala are immutable like in Define-and-Run frameworks, and interoperable with Scala like in Define-by-Run frameworks.

8.2 AD in a Functional Library

Reverse mode AD as a functional library was previously considered as impossible to implement without the ability to reflectively access and transform expressions associated with closures[Pearlmutter and Siskind 2008]. For example, if you want to create a `transform` function that returns the derivative for given function `f`:

```
def transform(f: Double => Double): Double => Double
```

Listing 29. Impossible transform function for AD

Obviously this `transform` function is impossible without the knowledge of the implementation of `f`.

Fortunately, in a statically typed language, the differentiable types and non-differentiable types should differ for type safety. The type signature of our AD function can use the differentiable type `DoubleLayer` instead of `Double`. It can be written as Listing 30:

```
def typeSafeTransform(f: Double => DoubleLayer): Double => SideEffects = {
    input: Double =>
  val tape = f(input).forward
  tape.backward(Do.now(1.0))
}
```

Listing 30. Type safe transform function for AD

Unlike[Pearlmutter and Siskind 2008]'s compiler primitive $\overleftarrow{J}$, our `typeSafeTransform` can use the additional methods on `DoubleLayer`. As a result, our `typeSafeTransform` can be implemented without reflection, as an ordinary Scala function, instead of a compiler primitive or a macro.

We also change the derivative type to an opaque monadic type `SideEffects`. Unlike numeric derivative, `SideEffects` can contain derivatives for more than one trainable variables, although this change exclude the ability of higher order numerical differentiation.

8.3 Portability

Our approach can be implemented in a library, which requires few advanced language features. Therefore, it can be ported to other languages that are not so powerful.

Our static DAGs are applicative, which can be built from normal function calls or overloaded operators without compiler-time transformation, as described in section 3.3.

Our direct style dynamic neural networks require only one uncommon language feature, which is !-notation, or direct style monadic expression, as described in section 3.1. The usage of this feature does not prevent porting our approach to other languages, because:

- The usage of !-notation is optional, as users of DeepLearning.scala can instead use **`for`** comprehension if they choose not to use !-notation.
- Direct style monadic expressions are available in Idris (!-notation), Haskell (do-notation) and F# (computational expressions). Our approach can be ported to those languages without a doubt.

- All callback functions of monadic data types, including `Do`, `Future` and `UnitContinuation` will never be re-evaluated by DeepLearning.scala more than once. Therefore, those monadic data types can be replaced to generators, coroutines or one-pass continuations, which has became a widely adopted feature in many mainstream languages, including ECMAScript, TypeScript, Go, Python, C#, C++20, Lua.
- For Java or other languages that do not support generators or coroutines, those !-notation can be replaced to manually written `flatMap` calls.

8.4 Related works

In this section, we will discuss other deep learning frameworks in statically typed languages.

Several AD libraries[Baydin et al. 2015a; Bischof et al. 1992; Griewank et al. 1996; Hascoët and Pascual 2013] written in Fortran, C++ or F# support AD via operator overloading or external preprocessor but do not scale to deep neural networks, either due to using forward mode or lacking the feature of multiple trainable variables.

Other deep learning frameworks in statically typed languages (including Scala binding of C++ frameworks)[Baydin and Pearlmutter 2016; Chen 2017; Intel 2016; Skymind 2017a; Zhao et al. 2017] do not support AD, instead, they only provide their high level computational graph APIs to compose predefined layers into neural networks. As a result, those frameworks do not have the ability to create fine-grained custom algorithms.

[Elliott 2018] presented an approach that unified compiler-time translation for AD. The approach requires a compiler plug-in that translates Haskell programs into categorical form, which gives the ability to hook into each function call. By providing different instances of type classes, those function calls can translated to differential functions of different modes of AD. Unfortunately, the compiler plug-in is only available in Haskell, thus the approach is unable to be implemented in other languages. In contrast, our approach requires no metaprogramming features, thus can be implemented in many mainstream languages, as explained in section 8.3.

[Wang et al. [n. d.]] discovered an approach to perform reverse mode AD in delimited continuations. Their approach is very simple: (1) In forward pass, a chain of delimited continuations is created by `shift` calls, which inject some hooks that contain side effects to update the derivatives. (2) In backward pass, hooks are executed in reverse order, triggered by `reset`. However, their approach directly perform side effects in hooks, and always executes both forward pass and backward pass sequentially. In contrast, side effects in our approach are encapsulated in tasks of monadic data types, and we also provide nondeterministic implementation of applicative operations on those task types, allowing for parallel execution of both the forward pass and backward pass.

9 CONCLUSION

DeepLearning.scala is the first library that achieves all the following goals without metaprogramming technique:

- static type safety
- purely functional interface
- reverse mode AD
- multiple trainable variables
- interoperable internal DSL
- dynamic neural network
- statically type checking

With the help of DeepLearning.scala, normal programmers are able to build complex neural networks from simple code. They still write code as usual, and the only difference is that the code

written in DeepLearning.scala is differentiable, which contains trainable variables that learn the knowledge.

GLOSSARY

computational graph is an asynchronous monadic data type that manages the life cycle of tapes, whose type is `Do[Tape[Data, Delta]]` . 5, 7, 11, 14–20, 22, 24, 25

differentiable expression is a composable expression that supports operator overloading, whose type is `DoubleLayer`, `FloatLayer`, `INDArrayLayer`, or other subtypes of `Layer`. After a differentiable expression is built, it can perform `forward` pass to create a differentiable computational graphs. . 3, 5, 6, 10, 16, 17, 25

differentiable function is a Scala function that returns a differentiable expression. It may represent a loss functions, a neural network or a subset of a neural network (e.g. a dense block in DenseNet[Iandola et al. 2014]) . 5, 10, 11, 15–17

trainable variable is a scalar or vector weight in a model, whose type is `DoubleWeight`, `FloatWeight` , `INDArrayWeight`, or other subtypes of `Weight` . 1, 3, 5, 10–12, 14–17, 20, 23–25

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