Abstract
Axon is a language that enables shape and rank inference for tensors in a Deep Learning graphs. It aims to make shapes implicit and inferred, in a similar manner to how types are implicit and inferred in many functional programming languages. Tensor dimensions are represented by expressions consisting of symbolic variables, constants, and arithmetic operators. Tensor shapes can be expressed as either a sequence of these dimension expressions, as a symbolic variable, or as an appending the dimensions of several other shapes. This allows complex constraints on shapes to be expressed.

Axon is functional in style, with a type system similar in to Standard ML, extended to include shape information. It provides a suite of built in operators over tensors, including pointwise arithmetic operators, maps, reduction, loops and user defined functions.

We describe a shape inference algorithm based on constraint solving which infers information about shapes, from both shape information provided by the programmer and the structure of the program. This allows fully automatic inference of the shapes of tensors for complex Deep Learning graphs.

This approach reduces programmer effort when specifying graphs, as tensor shapes are not explicit, allows composition of Deep Learning graphs while maintaining input and output tensor shape compatibility, and aids in automated error detection by identifying shape mismatches at runtime.

1 Introduction
Deep Learning models can be viewed as constrained functional programs on tensor domains, which only permit side effects or updates for certain types of models, and usually only during training. Tensors have a type and a shape: they are rectangular domains of simple element types. Requiring the programmer to deal with these shapes can add significant complexity to a language.

This paper describes shape and rank inference for tensors in a language we call Axon, which aims to make shapes implicit and inferred, in a similar manner to how types are implicit and inferred in many functional programming languages. Axon allows the individual dimensions of a tensor to be expressions consisting of symbolic variables, constants, and arithmetic operators, allowing complex constraints on shapes to be expressed. Furthermore, shapes can be expressed as either a sequence of these dimension expressions, as a symbolic variable, or as an appending the dimensions of several other shapes. This allows rank inference to be expressed using this shape appending.

An inference algorithm is also presented which infers information about shapes, from both shape information provided by the programmer and the structure of the program, via a set of rules for built-in operators. Our system allows the shapes involved in complex Deep Learning problems to be automatically inferred without need for the programmer to express the shape constraints or give concrete shapes which are potentially unknown until the shape of the inputs to the program are known. Shape information can be inferred from known shapes, or partial shapes, of program inputs and from the structure of the program itself. Automated error detection also aids programmers by identifying shape mismatches between the allowed shapes to an operation and inferred shapes.

The rest of the paper is structured as follows. Section 2 outlines the Axon language. Section 3 presents the syntax of shape expressions, section 4 describes how standard Hindley-Milner type inference [4, 7] is used to generate a set of shape constraints for the program and section 5 describes the algorithm used to solve sets of these shape constraints. Section 6 provides examples of shape inference in action and section 7 provides larger examples for commonly seen Deep Learning graphs. Section 8 discusses related work and section 9 presents our conclusions.

This paper makes the following contributions:
- A taxonomy of the kinds of shapes encountered in Deep Learning graphs, which we use to guide the design of the language.
- A functional programming language, which we call Axon. It allows a programmer to specify symbolic shapes for input and output tensors for a graph, which permit arithmetic expressions for the dimensions, and allows for rank inference by expressing shapes as the composition of sub-shapes.
- A constraint based solver for inferring shape information throughout a program, based on a set of shape inference rules. Initial constraints are generated based on the structure of a graph, and the rules are used to reduce these constraints to a fixed point, where either all shapes are known rank with constant dimensions, or are partially unknown allowing for runtime variable shape.
2 The Axon Language

The goal of Axon is to provide a language for easily writing Deep Learning graphs, in a target agnostic manner. It provides a high-level functional language for representing Deep Learning graphs, through the use of a suite of built-in deep learning operators. The Axon compiler includes a type inference algorithm, so that explicit types do not need to be specified by the programmer. Furthermore, an inference algorithm for shapes also removes the need for explicit tensor shapes to be specified by the programmer.

A simple graph that compute the pointwise sum and product of two inputs can be expressed in Axon as follows:

```
f = fn(x, y) {
  a = x + y;
  b = x * y;
  a, b
}
```

This program describes a graph called $f$ which takes two inputs $x$ and $y$ and produces two outputs $a$ and $b$. In Axon, all variables are tensors. These have an element type (with the usual primitive types including fixed size integers and floating point data types, and a shape.

Axon allows program decomposition into sub-graphs as in the following example:

```
g = fn(a, b) {
  a + b
};
f = fn(a, b) {
  g(a, b) + a;
}
```

This allows a program to be decomposed into smaller modular parts and reused. The type and shape inference algorithm allow for polymorphic types and shapes. For example, in the above graph, if $g$ were called from multiple places it could be called with different types and shapes.

Axon includes a suite of operators for performing Deep Learning computations. These include matrix multiplication, convolution, point-wise arithmetic operators, loops and more. The language includes a type specification for each built-in, which is used to infer types and shapes throughout the graph. Examples of these are given in Section 3.3.

3 Tensor Shapes

In this section we describe the shapes of tensors in the Axon language. Section 3.1 outlines a general taxonomy of shapes we use to guide our design and discussion. These are a general overview of the sorts of shapes that appear in Deep Learning graphs. In Section 3.2 we give the concrete syntax of shapes in the Axon. Examples of shape constraints are given in Section 3.3, which show how shape constraints are generated from the syntactic structure of a graph. The algorithm for then solving these constraints is given later, in Section 5.

3.1 Taxonomy of Shapes

Here we specify the general taxonomy of shapes we use to guide the design of our language. This taxonomy categorizes the possible tensor shapes based on their properties and constraints.

- **Concrete shapes**
  These are shapes of statically known constant rank whose dimensions are all statically known constants. For example $\left[\begin{array}{c}1\end{array}\right]$ denotes a scalar, $\left[\begin{array}{c}256\end{array}\right]$ denotes a one dimensional tensor of 256 elements, and $\left[\begin{array}{c}1024, 256\end{array}\right]$ denotes a two dimension tensor.

- **Symbolic dimensions**
  These extend concrete shapes by allowing individual dimensions to be symbolic expressions. The rank of the shape is still statically known. For example $\left[\begin{array}{c}x, y, 16\end{array}\right]$ is a three dimensional tensor whose inner two dimensions are symbolic variables. At runtime, $x$ and $y$ will be known, but at compile time their value is unknown.

- **Runtime dimensions**
  Here the rank is static, but the individual dimensions can depend on the computation.

- **Variable**
  Dimension values differ across the tensor. This allows, for example, ragged batches to be represented.

3.2 Syntax of Shapes

Figure 1 gives the syntax of shapes in Axon. The syntax of shapes is too complex for a succinct grammar, therefore the grammar given in Figure 1 generates some invalid shapes, which are further constrained by the shape construction rules given in Figure 2.

Shapes can be fixed, or variable, according to the dimension expressions they contain. The syntax of these expressions includes positive integer constants, symbolic variables and arithmetic operations and a “variable dimension” denoted *'. The * dimension expression (with no arguments) denotes a variable dimension, i.e. the number of elements in this dimension varies across the other dimensions in the tensor. This allows, for example, batches of variable length
sequences to be represented. The shape of a batch of 10 variable length sequences of 3-dimensional vectors would be denoted [10, *, 3].

The shape append construct @ allows for shapes to be expressed as many sub-shapes that are appended to one another. This allows shape constraints such as s@[n] which denotes a shape with a rank of at least one, where the outermost dimension has size n. This is how Axon provides rank inference. We have found from our experience that this append construct is able to represent the kinds of variable rank that we see in real Deep Learning graphs.

3.3 Example Shape Constraints

The following gives the types of commonly encountered deep learning operators. These type signatures are used by the shape inference to infer information about the shapes of inputs and outputs and to check that inputs and outputs to these operators are of a valid shape. When a graph is constructed, rules such as these are used to create a set of shape constraints that can then be solved to infer shape information about a graph. More details of how shape constraints are generated is given in Section 4, and the algorithm used to solve them is given in Section 5.

- Concatenation
  \( \tau[d]@s, \tau[d]@s \rightarrow \tau[(+d2)]@s \)
  This function takes two tensors which have shape \([d_1]@s\) and \([d_2]@s\), and concatenates them along their outermost dimension. This results in an output of shape \([(+d_1) d_2]@s\). The outermost dimension of the output has a size which is equal to the sum of the outermost dimensions of the inputs, and the rest of the dimensions are arbitrary but match the inputs.

- Matrix multiplication
  \( \tau[s[d_1, d_2], \tau[d_2, d_3]] \rightarrow \tau[d_1, d_3] \)
  This function takes a tensor of shape \(s[d_1, d_2]\) and a tensor of shape \(s[d_1, d_2]\) and produces an output tensor of shape \(s[d_1, d_3]\). s is the shape of the batch (i.e., the matrix multiplication operates on the outer two dimensions of the inputs, and the outer dimensions must be equal, and are denoted s). The outer dimensions of the output shape are \(d_1, d_3\), which expresses fact that the result has the shape of the first dimension of the first input, and the second dimension of the second input. Finally, the inputs share dimension expression \(d_2\) which expresses the need for the outer and inner dimensions of the two matrices to be equal.

- 2D Convolution in NCHW format
  \( \tau[n, c, h, w], \tau[k, c, r, s]) \rightarrow \tau[n, c, 1 + h - r, 1 + w - s] \)
  The shape of the output of a convolution is an arithmetic function of the shape of the inputs.
4 Shape Constraint Generation

Our approach extends Hindley-Milner type inference [2], using standard type unification with an additional rule which generates shape constraints. This rule is described in Section 4.1. From these generated shape constraints, a shape solver (based on unification) computes concrete shapes where possible from these shape constraints. This part of the algorithm is covered in detail in Section 5.

Given a program, which is functional in style and may be annotated with shapes by the programmer, Hindley-Milner style type inference and unification algorithms are used. This is done as part of the standard Hindley-Milner type inference algorithm. To infer information about shapes within a program, the shape solver discovers are then replaced in the types of the program. A shape solver is run over these constraints as part of the type inference algorithm.

4.1 Constraint Generation Rules

In order to infer information about shapes within a program, a set of shape constraints first needs to be generated for a program. This is done as part of the standard Hindley-Milner style type inference algorithm.

Unification is augmented to generate not only a type substitution for a pair of types, but also a set of type constraints. Whenever two tensor types involving shapes are unified, shape constraints are generated and added to the set. After unification is complete these shape constraint sets are solved using the shape solving algorithm presented in Section 5. This shape constraint generation and solving is done incrementally as part of the type inference algorithm.

The additional unification rules for tensor types are given in Figure 3. $G$ denotes the set of types to be unified (initially $G = \{t_1 = t_2\}$ where $t_1$ and $t_2$ are the two types being unified). $s$ denotes the set of shape constraints, initially $s = \emptyset$. If any rules match $(G, S)$ and generate a FAIL then unification fails. Unification finishes when none of the rules match anything in $(G, S)$. At this point, $G$ will contain a substitution from type variables to types, and $S$ will contain the set of shape constraints.

The first rule in Figure 3 just reorders the type so that type variables (denoted $a$) appear on the left hand side. The second rule generates a new shape constraint given two tensor types with shapes $s_1$ and $s_2$. The third rule causes unification to fail if a free type variable appears on both the left hand side (denoted $a$) or anywhere in the type on the left hand side (denoted $r$).

\[
\begin{align*}
\langle G \cup \{rs = a\}, S \rangle &\Rightarrow \langle G \cup \{a = rs\}, S \rangle \\
\langle G \cup \{t_1s_1 = t_2s_2\}, S \rangle &\Rightarrow \langle G \cup \{t_1 = t_2\}, S \cup \{s_1 = s_2\} \rangle \\
\langle G \cup \{a = rs\}, S \rangle &\Rightarrow FAIL \text{ if } a \in ftv(r)
\end{align*}
\]

Figure 3. Unification rules for tensor types to generate shape constraints

5 Shape Solver

Type inference, as described in Section 4 produces a set of shape constraints of the form:

\[
C = \{s_1 = s'_1, \ldots, s_n = s'_n\}
\]

The shape solver attempts to simplify this constraint set, and deduce concrete values for shapes where possible. As shapes can depend on runtime values, the shape solver may not be able to statically determine the value for all shape expressions. The solver uses an algorithm similar to unification.

The solve-shapes algorithm applies the following rules to the set of constraints until a fixed point is reached. Rules are matched on the syntax of shapes, where $a$ denote shape variables, $c$ denote integer constants, $s$ denotes shapes, $d$ denotes dimensions. $\hat{s}$ denotes both shapes and dimensions. Two shapes are equivalent ($\equiv$) if their syntax is identical. If FAIL is reached, the shape solver fails (as an invalid constraint has been found).

$C$ is the constraint set to be reduced. $C[\hat{s}/a]$ denotes the constraint set with all $a$ replaced with $\hat{s}$. $fsv(\hat{s})$ denotes the set of shape and dimension variables that are free in $\hat{s}$.

Basic Rules

These rules remove constraints that are tautologies, perform replacement of free shape variables that have been determined and emit an error when different constants are equated to each other in a constraint.

\[
\begin{align*}
C \cup \{s_1 = s_2\} &\Rightarrow C \text{ if } s_1 \equiv s_2 \\
C \cup \{a = \hat{s}\} &\Rightarrow C[\hat{s}/a] \cup \{a = \hat{s}\} \\
&\text{ if } a \in fsv(C) \text{ and } a \notin fsv(\hat{s}) \\
C \cup \{c_1 = c_2\} &\Rightarrow FAIL \text{ if } c_1 \neq c_2
\end{align*}
\]

Reordering

These rules reorder constraints with a constant on one side so that it is on the right hand side. These rules remove the
need for many symmetric rules later.

\[
\begin{align*}
& C \cup \{c = s\} \Rightarrow C \cup \{s = c\} \\
& C \cup \{c = a\} \Rightarrow C \cup \{a = c\} \\
& C \cup \{a = \ast\} \Rightarrow C \cup \{a = \ast\} \\
& C \cup \{(\text{op } d_1 \ d_2) = a\} \Rightarrow C \cup \{a = (\text{op } d_1 \ d_2)\} \\
& C \cup \{(d_1, \ldots, d_n) = a\} \Rightarrow C \cup \{a = [d_1, \ldots, d_n]\} \\
& C \cup \{s_1 @ \ldots @ s_n = a\} \Rightarrow C \cup \{a = s_1 @ \ldots @ s_n\}
\end{align*}
\]

Unpacking
These rules equate the shape expressions making up shapes of known rank.

\[
\begin{align*}
& C \cup \{[d_1, \ldots, d_n] = [d'_1, \ldots, d'_n]\} \\
& \Rightarrow C \cup \{d_1 = d'_1, \ldots, d_n = d'_n\} \\
& C \cup \{[d_1, \ldots, d_n] = [d'_1, \ldots, d'_m]\} \\
& \Rightarrow \text{FAIL if } n \neq m
\end{align*}
\]

Empty shapes
These rules assign the empty shape to shapes appended either side of a shape of known rank, where possible.

\[
\begin{align*}
& C \cup \{[d_1, \ldots, d_n] = s_1 @ \ldots @ s_j @ [d'_1, \ldots, d'_n]\} \\
& @ s_{j+1} \ldots @ s_m \\
& \Rightarrow C \cup \{[d_1, \ldots, d_n] = [d'_1, \ldots, d'_n], s_1 = [], \ldots, s_m = []\} \\
& C \cup \{s_1 @ \ldots @ s_j @ [d'_1, \ldots, d'_n]\} \\
& @ s_{j+1} \ldots @ s_m = [d_1, \ldots, d_n] \\
& \Rightarrow C \cup \{[d_1, \ldots, d_n] = [d'_1, \ldots, d'_n], s_1 = [], \ldots, s_m = []\}
\end{align*}
\]

Append Unpacking
These rules equate dimension expressions that are at the start and end of appended shapes.

\[
\begin{align*}
& C \cup \{s @ [d_1, \ldots, d_n] = s' @ [d'_1, \ldots, d'_m]\} \\
& \Rightarrow C \cup \{s @ [d_1, \ldots, d_{n-1}] = s' @ [d'_1, \ldots, d'_{m-1}], d_n = d'_m\} \\
& C \cup \{[d_1, \ldots, d_n] @ s = [d'_1, \ldots, d'_m] @ s'\} \\
& \Rightarrow C \cup \{[d_1, \ldots, d_n] @ s = [d'_1, \ldots, d'_m] @ s', d_1 = d'_1\}
\end{align*}
\]

Append Dimensionality
These rules check for shape appsends whose minimum rank is greater than a concrete shape that they are equal to.

\[
\begin{align*}
& C \cup \{s_1 @ \ldots @ s_n = [d_1, \ldots, d_m]\} \\
& \Rightarrow \text{FAIL if number of dimensions in } s_1, \ldots, s_n > m \\
& C \cup \{[d_1, \ldots, d_m] = s_1 @ \ldots @ s_n\} \\
& \Rightarrow \text{FAIL if number of dimensions in } s_1, \ldots, s_n > m
\end{align*}
\]

Simplification
These rules use the simp function to simplify shapes in the constraints.

\[
\begin{align*}
& C \cup \{s_1 = s_2\} \\
& \Rightarrow C \cup \{s'_1 = s'_2\} \\
& \text{where } s'_1 = \text{simp}(s_1), \ s'_2 = \text{simp}(s_2) \\
& \text{if } s_1 \neq s'_1 \text{ or } s_2 \neq s'_2
\end{align*}
\]

The simp function takes a shape, or a shape expression, and returns its canonical form. This algorithm is recursive over the syntax of shapes and shape expressions. It simplifies shapes, by computing operators of any constants, ordering variables by name inside arithmetic operators, removing empty shapes in shape appsends, and computing shape appsends where possible.

Arithmetic Simplification
These rules simplify arithmetic expressions.

\[
\begin{align*}
& C \cup \{(d \ c_1) = c_2\} \Rightarrow C \cup \{s = \frac{c_2}{c_1}\} \text{ if } c_2 \mod c_1 = 0 \\
& C \cup \{(d + c_1) = c_2\} \Rightarrow C \cup \{s = c_2 - c_1\} \text{ if } c_2 - c_1 > 0 \\
& C \cup \{(d - c_1) = c_2\} \Rightarrow C \cup \{s = c_1 + c_2\}
\end{align*}
\]

Partial Expression Simplification
This rule allows unsolvable expressions that equate to a constant to be replaced within other constraints.

\[
\begin{align*}
& C + \{(\text{op } s_1 \ s_2) = c\} \\
& \Rightarrow C[c/(\text{op } s_1 \ s_2)] + \{(\text{op } s_1 \ s_2) = c\} \\
& \text{if } (\text{op } s_1 \ s_2) \in C
\end{align*}
\]

6 Inference Examples
This section presents a set of example programs, and how shape inference can determine the shapes of their inputs and outputs, based on both shapes provided by the programmer and the structure of the program itself.

6.1 Basic Symbolic Constraints
The following Axon function performs matrix multiplication on a pair of square matrices of size n. The inputs have shape [n, n] and the return type is given name r. This example demonstrates how the output shape is inferred from the input shape, and the structure of the program:

```axon
fn (x : f32 [n, n], y : f32 [n, n]) : r (matmul(x, y))
```

The program uses the generalized matrix multiplication operator `matmul`, whose type specification is as follows, where `r` denotes the element type of the tensor:

\[
(r \ s@[d_1, d_2], \ r \ s@[d_3, d_4]) \rightarrow r \ s@[d_1, d_3]
\]
The set of shape constraints, generated by type checking this program, are:

\[
\begin{align*}
s & @ [d_1, d_2] \equiv [n, n] \\
\text{and} & \quad s @ [d_2, d_3] \equiv [n, n] \\
\text{and} & \quad s @ [d_1, d_3] = r
\end{align*}
\]

The first two constraints match the empty shapes rule, which assigns \( s \) to be the empty shape. The constraints are now:

\[
\begin{align*}
[d_1, d_2] & = [n, n] \quad s @ [d_1, d_3] = r \\
[d_2, d_3] & = [n, n] \quad s = \emptyset
\end{align*}
\]

The unpacking rule for shapes of known rank now applies to the first two constraints, giving:

\[
\begin{align*}
d_1 & = n \quad s @ [d_1, d_3] = r \\
d_2 & = n \quad s = \emptyset \\
d_3 & = n
\end{align*}
\]

The reordering rule matches the fourth constraint, giving:

\[
\begin{align*}
d_1 & = n \\
r & = s @ [d_1, d_3] \\
ds & = \emptyset
\end{align*}
\]

The basic rule now matches constraint five, replacing \( s \) with the empty shape in constraint four:

\[
\begin{align*}
d_1 & = n \quad r = \emptyset @ [d_1, d_3] \\
d_2 & = n \quad s = \emptyset \\
d_3 & = n
\end{align*}
\]

The basic rule also matches constraints one and three, replacing \( d_1 \) and \( d_3 \) in constraint four:

\[
\begin{align*}
d_1 & = n \\
r & = \emptyset @ [n, n] \\
ds & = \emptyset
\end{align*}
\]

Shape simplification then removes the empty shape append in constraint four:

\[
\begin{align*}
d_1 & = n \\
r & = [n, n] \\
ds & = \emptyset
\end{align*}
\]

Shape inference is now complete, as no rules match any of the constraints. The return shape has been correctly inferred as \([n, n]\). Furthermore, the remaining constraints form a shape substitution, mapping variables to shapes. The shapes for the arguments and return from the \texttt{matmul} call can then be found by applying this substitution to the type of \texttt{matmul}:

\[
(\tau[n,n], \tau[n,n]) \rightarrow \tau[n,n]
\]

### 6.2 Arithmetic Expressions for Shapes

The following program performs a 2d convolution of an 8x8 filter over an input of unknown shape \( i \). The result shape is known. This example demonstrates that shape inference can infer the shape of the input from the shape of the output.

```plaintext
fn (x : t i, f : t [4,8,8,8]) : t [4,8,1024,256] { 
  conv(x, f)
}
```

The set of type constraints generated by type checking is:

\[
\begin{align*}
[n,c,h,w] & = i \\
[k,c,r,s] & = [4,8,8,8] \\
[n,c, (+ 1 (- h r)), (+ 1 (- w s))] & = [4,8,1024,256]
\end{align*}
\]

The second and third constraints matches the unpacking rule for shapes of known rank, which gives the following set of constraints:

\[
\begin{align*}
[n,c,h,w] & = i \quad r = 8 \\
n & = 4 \quad s = 8 \\
k & = 4 \quad (+ 1 (- h r)) = 1024 \\
c & = 8 \quad (+ 1 (- w s)) = 256
\end{align*}
\]

Reordering reorders the first constraint:

\[
\begin{align*}
i & = [4,8,h,w] \quad r = 8 \\
n & = 4 \quad s = 8 \\
k & = 4 \quad (+ 1 (- h 8)) = 1024 \\
c & = 8 \quad (+ 1 (- w 8)) = 256
\end{align*}
\]

The simplification algorithm applied to the arithmetic expressions reorders them into canonical form:

\[
\begin{align*}
i & = [4,8,h,w] \quad r = 8 \\
n & = 4 \quad s = 8 \\
k & = 4 \quad (+ (- h 8) 1) = 1024 \\
c & = 8 \quad (+ (- w 8) 1) = 256
\end{align*}
\]

The arithmetic simplification rule then produces:

\[
\begin{align*}
i & = [4,8,h,w] \quad r = 8 \\
n & = 4 \quad s = 8 \\
k & = 4 \quad (- h 8) = 1024 \\
c & = 8 \quad (- w 8) = 255
\end{align*}
\]
And again:
\[
\begin{align*}
i &= [4, 8, h, w] & r &= 8 \\
n &= 4 & s &= 8 \\
k &= 4 & h &= 1031 \\
c &= 8 & w &= 263
\end{align*}
\]

The basic rule for variable replacement then produces:
\[
\begin{align*}
i &= [4, 8, 1031, 263] & r &= 8 \\
n &= 4 & s &= 8 \\
k &= 4 & h &= 1031 \\
c &= 8 & w &= 263
\end{align*}
\]

And shape inference is complete. The shape of the input has been inferred as \([4, 8, 1031, 263]\).

6.3 Discovering Shapes of Inputs
The shape inference algorithm allows the shapes of unknown inputs to be inferred from other information in the program. For example, consider the following example. The type signature of \(\text{max}\) determines the shape of the second input, given the shape of the first input. This demonstrates that shape information can be inferred not only “forward” from input shapes to output shapes, but also “in reverse” back to the inputs.

\[
\text{softmax} = \text{fn} (e : f32 s) \rightarrow \begin{align*}
y &= \text{reduce}(\text{max}, -\text{inf}, e) \\
z &= \text{exp}(x - y) \\
z / \text{reduce}(+, 0f, z)
\end{align*}
\]

Here the shape of \(e\) is inferred to also be a scalar \(f32\), due to the other input being a scalar \(f32\) and the type signature for \(\text{max}\). The return type of the function is also inferred to be \(f32\).

6.4 Partial Shape Information
Sometimes there is not enough information to determine concrete shapes for all parts of a program. Our shape inference algorithms allows partial shape information to be discovered, for example consider the following \(\text{softmax}\) program:

\[
\begin{align*}
\text{softmax} &= \text{fn} (x : f32 s) \rightarrow \begin{align*}
y &= \text{reduce}(\text{max}, -\text{inf}, x) \\
z &= \text{exp}(x - y) \\
z / \text{reduce}(+, 0f, z)
\end{align*}
\end{align*}
\]

No shape information is given in the type of the input (it is just denoted \(s\)), however type information can be determined from the operations contained within the program. Running shape inference on this program yields the following type for the \(\text{softmax}\) function:

\[
f32 [a]@b \rightarrow f32 [a]@b
\]

Shape inference has discovered, based on the type signatures of the operations within the program, that it can accept any input with a rank of at least one (the first dimension is denoted \(a\)) and arbitrary outer dimensions (denoted \(b\)). Furthermore, the output of the function is also inferred to have the same shape as the input.

7 Example Graphs
This section presents example graphs, and how shape inference can determine the shapes of their inputs and outputs.

7.1 Attention
A commonly used computation in machine learning models is attention [10]. This can be written as the following mathematical function:

\[
\text{attention}(Q, K, V) = \text{softmax} \left( \frac{QK^T}{\sqrt{d_k}} \right) V
\]

This can then be implemented in Axon as follows:

\[
\begin{align*}
\text{softmax} &= \text{fn} (e : t [m,n]) \rightarrow \begin{align*}
y &= \text{reduce}(\text{max}, -\text{inf}, e) \\
z &= \text{exp}(e) \\
s &= \text{map}(\text{fn} (a) \rightarrow \begin{align*}
\text{reduce}(+, 0f, a) \\
\text{transpose}(a)
\end{align*}, \text{transpose}(e))
\end{align*}
\end{align*}
\]

Attention can then be implemented in Axon as follows:

\[
\begin{align*}
\text{attention} &= \text{fn} (Q, K, V) \rightarrow \begin{align*}
&\text{matmul}(\text{softmax}(\text{matmul}(Q, \text{transpose}(K))), V)
\end{align*}
\end{align*}
\]

In this program, all of the types and shapes are implicit and unconstrained, except for the input to the \(\text{softmax}\) function, which has type \(t[m,n]\). This type annotation constrains the input to be of any element types, with a shape which is two dimensional, with dimensions \(m\) and \(n\) respectively.

Axon includes rules for generating shape constraints for all of the built-in functions used in this program, such as \(\text{matmul}\), \(\text{transpose}\) and \(\text{map}\) as described in Section 3.3. These rules generate a set of constraints, which when solved give the following type and shape signature for the attention function:

\[
t[a,b], t[c,b], t[c,d] \rightarrow t[a,d]
\]

7.2 Loops and Scans
Loops and scans, as used in LSTM models [5], can be written in Axon as follows:

\[
h_{out}, y = \text{loop}(h_{in}, \text{cell}, x)
\]

where \(\text{cell}\) is a function that takes the current state and outputs the next state, \(x\) is the input tensor, \(h_{in}\) is the initial
hidden state, \( h_{\text{out}} \) is the final hidden state and \( y \) is the output tensor.

This loop construct can be used to write an LSTM as follows, by simply specifying the appropriate cell function for the LSTM:

```plaintext
cell = fn (state : (t s1, t s2), y : t s3) {
    h1, c1 = state;
    hnext, cnext = lstmStep(
        y, h1, c1,
        W_i, W_f, W_o, W_c,
        R_i, R_f, R_o, R_c,
        B_i, B_f, B_o, B_c);
    (hnext, cnext), cnext
};
loop((h, c), cell, x)
```

As with the attention example, most of this program is left with unconstrained types and shapes. The only requirement is that the inputs to the cell function are a tuple of two tensors, and a tensor. In this example the shape solver will determine that the output of the loop has the same shape as the initial input tensor \( x \), and given the shape of \( x \), constrains the cell function to have the correct shapes. Namely, that \( s1, s2 \) and \( s3 \) should be equal to the shape of \( x \).

### 7.3 Recurrent Neural Networks

Bidirectional recurrent neural networks can be written in Axon as follows:

```plaintext
bidir = fn (a, b, c, d, s) {
    _, x = loop(a, b, s);
    _, y = loop(c, d, reverse(s));
    concat(x, reverse(y))
};
Y = bidir(s0, A, s0', A', X);
```

This uses the same loop construct as the LSTM example previously.

Similarly, residual recurrent neural networks can be written in Axon as follows:

```plaintext
residual = fn (a, b, s) {
    r = loop(a, b, s);
    r + s
};
X1 = residual(..., LSTM1, X0);
X2 = residual(..., LSTM2, X1);
```

### 8 Related Work

Roesch et al. [9] describe RelayIR – an intermediate representation for deep learning. Similarly to Axon, RelayIR is a functional statically typed language aimed at deep learning problems. In contrast to our work, it uses a dependent type system to allow shapes to be represented by expressions. Our approach instead extends the language of shapes to include arithmetic expressions, shape appending and other constructs in order to allow complex shapes to be represented.

As far as we are aware there are no other related works for deep learning in the literature, that use a constraint based methodology to infer shape information in graph programs.

Frameworks, such as TensorFlow [1] and Pytorch [8] can propagate shape information at graph construction time but do not use an approach that allows shape information to be inferred from outputs to inputs.

The MAGICA project [6] explores shape inference for MATLAB programs, using a symbolic evaluation approach, based on the algebraic properties of MATLAB. They use it to identify redundant shape array checks in MATLAB programs in order to reduce execution overheads at runtime.

Garg et al. [3] describe an approach that uses runtime information to perform shape inference on APL-like languages for just-in-time compilation. In contrast, our inference algorithm can be applied both statically at compile time, to infer potentially partial shape information, and again at runtime (if required) once the shapes of graph inputs are known.

### 9 Conclusions

This paper presents an algorithm for generating and solving shape constraints for Deep Learning graphs with dynamic shapes. This algorithm allows either fully static or partially static shapes to be discovered within a program, based on shape information provided by the programmer, and the structure of the graph. These shapes can include arithmetic expressions for their individual dimensions, and can also vary in rank. This is done using a fully automated shape constraint solver.
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