Efficient Differentiable Programming in a Functional Array-Processing Language

AMIR SHAIKHHA, EPFL, Switzerland
ANDREW FITZGIBBON, Microsoft HoloLens, United Kingdom
DIMITRIOS VYTINIOTIS, Microsoft Research, United Kingdom
SIMON PEYTON JONES, Microsoft Research, United Kingdom
CHRISTOPH KOCH, EPFL, Switzerland

We present a system for the automatic differentiation of a higher-order functional array-processing language. The core functional language underlying this system simultaneously supports both source-to-source automatic differentiation and global optimizations such as loop transformations. Thanks to this feature, we demonstrate how for some real-world machine learning and computer vision benchmarks, the system outperforms the state-of-the-art automatic differentiation tools.

... in the summer of 1958 John McCarthy decided to investigate differentiation as an interesting symbolic computation problem, which was difficult to express in the primitive programming languages of the day. This investigation led him to see the importance of functional arguments and recursive functions in the field of symbolic computation. From Norvig [38, p248].

1 INTRODUCTION

Functional programming (FP) and automatic differentiation (AD) have been natural partners for sixty years, and major functional languages all have elegant automatic differentiation packages [6, 17, 29]. With the increasing importance of numerical engineering disciplines such as machine learning, speech processing, and computer vision, there has never been a greater need for systems which mitigate the tedious and error-prone process of manual coding of derivatives. However the popular packages (TensorFlow, CNTK) all implement clunky (E)DSLs in procedural languages such as Python and C++. Why? One reason is that the FP packages are slower than their imperative counterparts, by many orders of magnitude [48], because modern applications depend heavily on array processing, with vectors, matrices, and tensors as the canonical datatypes. In contrast, AD for FP has generally handled only scalar workloads efficiently [29].

Our key contribution in this paper is to take a recently introduced F# subset designed for efficient compilation of array-processing workloads, and to augment it with vector AD primitives, yielding a functional AD tool that is competitive with the best C/C++ and Fortran tools on many benchmarks, and considerably faster on others.

1.1 The problem we address

Automatic differentiation is one of the main techniques for automating the process of computing derivatives. This technique systematically applies the chain rule, and evaluates the derivatives for the primitive arithmetic operations (such as addition, multiplication, etc.). One of the main advantages of automatic differentiation over its main competitive technique,
symbolic differentiation, is the constant-time overhead of the differentiated program with respect to the original code. Symbolic differentiation can lead to code explosion if one is not careful about sharing, and requires a closed-form representation of the programs [6].

There are two approaches for implementing AD. Forward-mode AD computes the derivative part (tangent part) alongside the original computation while making a forward pass over the program. Reverse-mode AD makes a forward pass to compute the original part of the program, followed by a backward pass for computing the derivative part (adjoint part). We present these two techniques through an example.

**Example.** Consider the function \( f(x_1, x_2) = \ln(x_1) + \sin(x_2) \), for which we would like to compute the partial derivatives with respect to \( x_1 \) at point \( x_1 = 1 \) and \( x_2 = 3 \). First let us name each intermediate expression with a variable \( v_i \):

\[
\begin{align*}
    f(x_1, x_2) &= \text{let } v_1 = \ln(x_1) \\
    &\text{let } v_2 = \sin(x_2) \\
    &\text{let } y = v_1 + v_2
\end{align*}
\]

This function is computed as follows:

\[
\begin{align*}
    v_1 &= \ln(1) = 0 \\
    v_2 &= \sin(3) = 0.1411 \\
    y &= 0 + 0.1411 = 0.1411
\end{align*}
\]

To compute the derivative of this function using the forward-mode AD, we associate the derivative \( \frac{\partial v_i}{\partial x_1} + \frac{\partial v_i}{\partial x_2} \) to each variable \( v_i \). As we are computing the partial derivative of \( f \) with respect to \( x_1 \), we have \( x_1 = 1 \) and \( x_2 = 0 \). By applying the chain rule, the evaluation trace for the derivative of this function is as follows:

\[
\begin{align*}
    \frac{\partial}{\partial x_1} &\frac{\partial v_1}{\partial x_1} = \frac{\partial}{\partial x_1} \frac{x_1}{x_1} = 1 \\
    \frac{\partial}{\partial x_2} &\frac{\partial v_2}{\partial x_2} = \frac{\partial}{\partial x_2} \frac{\sin(x_2)}{\sin(x_2)} = 0 \\
    \frac{\partial}{\partial x_1} &\frac{\partial y}{\partial v_1} = \frac{\partial}{\partial x_1} (v_1 + v_2) = 1 + 0 = 1 \\
    \frac{\partial}{\partial x_2} &\frac{\partial y}{\partial v_2} = \frac{\partial}{\partial x_2} (v_1 + v_2) = 1 + 0 = 1 \\
\end{align*}
\]

To compute the derivative of this function using the reverse-mode AD, we associate the adjoin term \( \frac{\partial y}{\partial v_i} \) to each variable \( v_i \). As a result, if we are interested in computing the partial derivative of function \( f \) with respect to \( x_1 \), we have to compute the value of \( \frac{\partial}{\partial x_1} \). To do so, we have to apply the chain rule in the reverse order, leading to the following execution trace:

\[
\begin{align*}
    \frac{\partial y}{\partial v_1} &= 1 \\
    \frac{\partial y}{\partial v_2} &= 1 \\
    \frac{\partial y}{\partial x_2} &= \frac{\partial v_2}{\partial x_2} = 1 \times \cos(3) = -0.9899 \\
    \frac{\partial y}{\partial x_1} &= \frac{\partial v_1}{\partial x_1} = 1 \times 1 = 1 \\
\end{align*}
\]

\( \Delta \)
Efficient Differentiable Programming in a Functional Array-Processing Language

\[
\begin{aligned}
\left. \frac{\partial f}{\partial x} \right|_a &= \frac{\partial f}{\partial x_1} a_1 + \frac{\partial f}{\partial x_2} a_2 + \cdots + \frac{\partial f}{\partial x_m} a_m \\
\end{aligned}
\]

Fig. 1. The Jacobian Matrix of a Function. Forward-mode AD computes a column of this matrix, whereas the reverse-mode AD computes a row of this matrix. \( d\tilde{f} \) computes the full Jacobian matrix using a vectorized variant of the forward-mode AD.

Forward and reverse mode compute a column and a row, respectively, of the full Jacobian matrix \( \mathbf{J} \) at each invocation. 1 More precisely, for a function with an input vector of size \( m \) and an output vector of size \( n \), the forward mode approach computes a column vector of size \( n \), and the reverse mode computes a row vector of size \( m \) (see Figure 1).

From a different point of view, for a given function \( f \) with an input vector parameter \( a \), forward-mode AD produces the function \( df \), where

\[
df \ a \ b = \mathbf{J} |_a \cdot b
\]

In the case of passing a one-hot vector as \( b \), where only the \( i^{th} \) element is one, the forward-mode AD computes the \( i^{th} \) column of the full Jacobian matrix. Similarly, for the same function, the reverse-mode AD produces the function \( bf \), where

\[
bf \ a \ c = \mathbf{J} |_a^T \cdot c
\]

This expression computes the \( j^{th} \) row of the full Jacobian matrix, if \( c \) is a one-hot vector with a single one at the \( j^{th} \) position and zeros elsewhere.

For a class of optimization problems, such as various computer vision problems using the Levenberg-Marquardt algorithm [31, 34, 35], one is required to compute the full Jacobian matrix. In such cases, neither of the two techniques perform efficiently.

To compute the full Jacobian matrix, both forward and reverse-mode techniques must iterate either over the columns or the rows of the Jacobian matrix, respectively. Given that both approaches have a constant overhead over the original computation, the forward mode technique is more efficient for computing the full Jacobian matrix when \( n \gg m \), whereas the reverse mode AD is more efficient when \( m \gg n \), an uneasy choice. Moreover:

- By carefully examining the body of the loops needed for computing the full Jacobian matrix, one can observe that many computations are loop-invariant and are unnecessarily performed multiple times. Thus, there is a lost opportunity for loop-invariant code motion for hoisting such expressions outside the loop, thus improving the performance (cf. the Bundle Adjustment experiment in Section 5).
- Furthermore, while the result of automatic differentiation is known to only have by a constant factor more arithmetic operations than the original program, the constant can be significant; this overhead can have a dramatic impact on the run-time performance in practice. More specifically, in applications involving the manipulation of vectors, many

\[1\] \( \mathbf{J} |_a \) is a matrix consisting of partial derivatives of the output elements of function \( f \) with respect to the elements of the input vector at point \( a \).
intermediate vectors are allocated that can be removed. The optimization for eliminating such intermediate vectors is known as deforestation [14, 19, 51, 54] or loop fusion in the functional programming community. This optimization opens the door for many other optimizations such as turning loops iterating over sparse vectors with a single non-zero element into a single statement (cf. Example 4 in Section 4).

1.2 Our contributions

In this paper, we present a novel automatic differentiation technique based on forward mode, which combines the benefits of both forward and reverse mode in many cases, and which, even for cases that require computing the full Jacobian matrix, outperforms both techniques. The key idea behind our technique is that we use a vector-aware programming language, in which the loops required for constructing the full Jacobian matrix are exposed to the compiler. Thus, the compiler can employ global optimization techniques such as loop-invariant code motion and loop fusion for simplifying the differentiated programs.

Example 1. Assume that we have a matrix \( M \) and two vectors \( u \) and \( v \) (which are represented as row matrices and are independent of \( M \)). Based on matrix calculus one can prove that
\[
\frac{\partial (uMv^T)}{\partial M} = u^Tv.
\]
However, computing the differentiated version of this function using forward-mode AD tools requires multiple iterations over the differentiated program for every element in the matrix \( M \). By using the reverse-mode AD, one can invoke the differentiated function only once, and the adjoin parts of the input matrix \( M \) will be filled in. We show in Section 4 that \( \tilde{d}F \) derives the gradient of this expression with respect to \( M \), resulting in an expression equivalent to \( u^Tv \). This removes the need for multiple iterations over the differentiated program for each element of matrix \( M \), in contrast to the existing AD tools based on the forward-mode AD technique.

The contributions of this paper are summarized as follows:

- We present \( \tilde{F} \), a higher-order functional array-processing language in Section 2.1. This language can be efficiently compiled into low-level C code with efficient memory management. Then, we present \( \tilde{M} \), a linear algebra DSL inspired by MATLAB, embedded [26] in this language in Section 2.2.
- Then, we show the differentiation programming capabilities provided by \( \tilde{F} \). First, Section 3.1 shows the high-level API exposed in \( \tilde{F} \) for performing various matrix derivatives such as scalar derivatives, gradients, and Jacobians. Then, we show transformation rules for performing source-to-source automatic differentiation of \( \tilde{F} \) expressions in Section 3.2.
- Afterwards, we show how \( \tilde{d}F \) produces efficient differentiated programs by introducing several global optimizations such as loop-invariant code motion, loop fusion, and partial evaluation, as well as generating C code with efficient stack-discipline memory management in Section 4.
- Finally, using several micro benchmarks and several functions used in machine learning and computer vision workloads, we show how \( \tilde{d}F \) outperforms the state-of-the-art AD techniques in Section 5.

2 OVERVIEW

In this section, we start with an overview of the compilation process in \( \tilde{d}F \), which is shown in Figure 2. This figure demonstrates the position of \( \tilde{d}F \) with respect to existing AD tools. \( \tilde{d}F \) starts from a program written in a high-level linear algebra DSL, called \( \tilde{M} \) (Section 2.2). This program is lowered into its implementation in a higher-order functional language with array
Efficient Differentiable Programming in a Functional Array-Processing Language

Fig. 2. Compilation process in $\tilde{\mathcal{F}}$ and other AD systems. The solid arrows correspond to the pipeline used in $\tilde{\mathcal{F}}$.

support, called $\tilde{\mathcal{F}}$ (Section 2.1). If a part of the program requires computing differentiation (which are specified by using high-level differentiation API exposed by $\tilde{\mathcal{F}}$, as mentioned in Section 3.1) $\tilde{\mathcal{F}}$ uses AD transformation rules (Section 3.2) for transforming the involved expressions into their differentiated form. Finally, after applying several simplifications such as loop fusion, partial evaluation, data layout transformation, etc. (Section 4) the differentiated program is transformed into low-level C code. The generated C code uses efficient stack-discipline memory management by using the destination-passing style (DPS) technique [44].

Next, we present the core functional language used in $\tilde{\mathcal{F}}$, on top of which we define source-to-source AD transformation and simplification rules.

2.1 $\tilde{\mathcal{F}}$

$\tilde{\mathcal{F}}$ (we pronounce it F smooth) is a subset of F#, an ML-like functional programming language. It is designed to be expressive enough to make it easy to write array-processing workloads, while simultaneously being restricted enough to be able to define automatic differentiation rules and allow it to be compiled to code that is as efficient as hand-written C, with very simple and efficient memory management [44].

Figure 3 shows the abstract syntax (parentheses can be used as necessary), type system, and several built-in functions of $\tilde{\mathcal{F}}$. In addition to the usual $\lambda$-calculus constructs (abstraction, application, and variable access), $\tilde{\mathcal{F}}$ supports let binding and conditionals.

$\tilde{\mathcal{F}}$ supports array programming by defining the following built-in functions: build for producing arrays; ifold for iteration for a particular number of times (from 0 to $n$-1) while
A. Shaikhha et al.

$$e ::= e \mid \text{fun } x \rightarrow e \mid x \quad \text{Application, Abstraction, and Variable Access}$$

| n | i | N | c | let x = e in e | if e then e else e |
|---|---|---|---|----------------|----------------|

$$T ::= M \quad \text{(Non-Functional) Expression Type}$$

| T | T ⇒ T | n | i | N | c | let x = e in e | if e then e else e |
|---|---|---|---|---|---|----------------|----------------|

$$M ::= \text{Num} \quad \text{Numeric Type}$$

| M | M × M | M | Bool | Num | Index | Card |
|---|---|---|---|---|---|---|

$$\text{Num ::= Double} \mid \text{Index} \mid \text{Card} \quad \text{Scalar, Index, and Cardinality Type}$$

**Typing Rules:**

\[
\begin{align*}
(T\text{-App}) & \frac{e_1 : T_1 \Rightarrow T_2 \ e_2 : T_1}{e_1 \ e_2 : T_2} \\
(T\text{-Abs}) & \frac{\Gamma \vdash \text{fun } x \rightarrow e : T_1 \Rightarrow T_2}{\Gamma \vdash \text{fun } x \rightarrow e : T} \\
(T\text{-Var}) & \frac{\Gamma \vdash x : T_1}{\Gamma \vdash x : T_2} \\
(T\text{-Let}) & \frac{\Gamma \vdash e_1 : T_1 \ \Gamma, x : T_1 \vdash e_2 : T_2}{\Gamma \vdash \text{let } x = e_1 \ \text{in } e_2 : T_2} \\
(T\text{-If}) & \frac{\Gamma \vdash e_1 : \text{Bool} \ \Gamma \vdash e_2 : M \ \Gamma \vdash e_3 : M}{\Gamma \vdash \text{if } e_1 \text{ then } e_2 \text{ else } e_3 : M}
\end{align*}
\]

**Scalar Function Constants:**

\[
\begin{align*}
+ | - | \times | \div | ^{} : \text{Num, Num } \Rightarrow \text{Num} \\
\sin | \cos | \tan | \ldots : \text{Num } \Rightarrow \text{Num} \\
\log | \exp : \text{Num } \Rightarrow \text{Num} \\
&& | \lvert | \rvert : \text{Bool } \Rightarrow \text{Bool} \\
\text{!} : \text{Bool } \Rightarrow \text{Bool}
\end{align*}
\]

**Vector Function Constants:**

\[
\begin{align*}
\text{build} : \text{Card } \Rightarrow (\text{Index } \Rightarrow M) \Rightarrow \text{Array}<M> \\
\text{get} : \text{Array}<M> \Rightarrow \text{Index } \Rightarrow M \\
\text{ifold} : (M \Rightarrow \text{Index } \Rightarrow M) \Rightarrow M \Rightarrow \text{Card } \Rightarrow M \\
\text{length} : \text{Array}<M> \Rightarrow \text{Card}
\end{align*}
\]

**Pair Function Constants:**

\[
\begin{align*}
\text{pair} : M_1 \Rightarrow M_2 \Rightarrow M_1 \times M_2 \\
\text{fst} : M_1 \times M_2 \Rightarrow M_1 \\
\text{snd} : M_1 \times M_2 \Rightarrow M_2
\end{align*}
\]

**Syntactic Sugar:**

\[
\begin{align*}
e_0[e_1] & = \text{get } e_0 \ e_1 & \text{Matrix} & = \text{Array}<\text{Array}<\text{Double}> > \\
(e_0, e_1) & = \text{pair } e_0 \ e_1 & \text{DoubleD} & = \text{Double } \times \text{Double} \\
e_1 \ bop \ e_2 & = \ bop \ e_1 \ e_2 & \text{VectorD} & = \text{Array}<\text{Double } \times \text{Double}> \\
\text{Vector} & = \text{Array}<\text{Double}> & \text{MatrixD} & = \text{Array}<\text{Array}<\text{Double } \times \text{Double}> >
\end{align*}
\]

Fig. 3. The syntax, type system, and function constants of the core $\tilde{F}$. maintaining a state across iterations; $\text{length}$ to get the size of an array; and $\text{get}$ to index an array.

One of the key features of $\tilde{F}$ is its support for both source-to-source automatic differentiati-
ation and global optimizations such as loop-invariant code motion and loop fusion in the same time. The transformations required for automatic differentiation are presented in Section 3.2, and the ones for optimization and simplification are shown in Section 4.

Next, we show how a Linear Algebra DSL can be defined on top of $\tilde{F}$.

2.2 $\tilde{M}$

$\tilde{M}$ is a functional Linear Algebra DSL, mainly inspired by MATLAB and R, programming languages which are heavily used by data analysts. By providing high-level vector and
Efficient Differentiable Programming in a Functional Array-Processing Language

| Matlab   | R         | NumPy  | \(\tilde{M}\) |
|---------|-----------|--------|-------------|
| A * B   | A %*% B   | A.dot(B) | matrixMult A B |
| A + B   | A + B     | A + B   | matrixAdd A B |
| A'      | t(A)      | A.T     | matrixTranspose A |
| ones(n, m) | matrix(1, n, m) | ones((n, m)) | matrixOnes n m |
| zeros(n, m) | matrix(0, n, m) | zeros((n, m)) | matrixZeros n m |
| eye(n)  | diag(n)   | eye(n)  | matrixEye n |

Table 1. Equivalent operations in Matlab, R, NumPy, and \(\tilde{M}\).

matrix operations, \(\tilde{M}\) frees the users from low-level details and enables them to focus on the algorithmic aspects of the problem in hand.

\(\tilde{M}\) is an embedded DSL (EDSL) \([26]\) in \(\tilde{F}\); it is defined as a library on top of \(\tilde{F}\). Figure 4 demonstrates a subset of \(\tilde{M}\) operations which are defined as functions in \(\tilde{F}\). This DSL is expressive enough for constructing vectors and matrices, elementwise-operations, accessing a slice of elements, reduction-based operations (computing the sum of vector elements), matrix transpose, and matrix multiplication. Supporting more sophisticated operations such as matrix determinant and matrix decomposition is beyond the scope of the current paper, and we leave it for the future. As discussed before, \(\tilde{M}\) is inspired by MATLAB and R. As a result, there is a mapping among the constructs of \(\tilde{M}\) and these matrix-based languages. Hence, it is easily possible to translate a program written in one of these languages to \(\tilde{M}\). Table 1 demonstrates the mapping among a subset of the constructs of MATLAB, R, NumPy and \(\tilde{M}\).

Example 1 (Continued). The matrix expression \(u M v^T\) is expressed as the following function in \(\tilde{M}\):

```haskell
let f = fun u M v ->
    let um = vectorToMatrix u
    let vt = matrixTranspose (vectorToMatrix v)
    let m = matrixMult um (matrixMult M vt)
    m[0][0]
```

The last expression is for accessing the single scalar element of a \(1 \times 1\) matrix.

△

3 DIFFERENTIATION

In this section, we show the differentiation process in \(d\tilde{F}\). First, we start by the high-level API exposed by \(d\tilde{F}\) to the end users. Then, we show how \(d\tilde{F}\) uses automatic differentiation behind the scenes for computing derivatives. Finally, we present the optimizations offered by \(d\tilde{F}\), and we demonstrate how \(d\tilde{F}\) can use these optimizations to deduce several matrix calculus identities.

3.1 High-Level API

For computing the derivative of an arbitrary function, \(d\tilde{F}\) provides the `deriv` construct. This construct can be better thought of as a macro, which is expanded during compilation time. The expanded expression includes the expression of the original computation, which is given as the first argument (and can be an arbitrary scalar, vector, or matrix expression), and
the derivative of this expression with respect to the variable given as the second argument, referred to as the independent variable. Note that one can easily compute the derivative of an expression with respect to a list of free variables by multiple invocation of the deriv construct.

Algorithm 1 shows a pseudo-code implementation of the deriv construct. First, deriv constructs a lambda function which has the free variables of the given expression as its input parameters (cf. line 6). This function is given as input to source-to-source automatic differentiation for computing the derivative (cf. line 8). The differentiated function is applied to the dual number encoding of all the free variables (cf. lines 5-8). If the free variable is different than the input variable with respect to which we are differentiating (i.e., the independent variable), the derivative part is a zero scalar, vector, or matrix (cf. lines 26-33). Otherwise, the derivative part is a one-hot encoding scalar, vector, or matrix (cf. lines 35-42).

Fig. 4. A subset of $\overline{M}$ constructs defined in $\overline{F}$.
Efficient Differentiable Programming in a Functional Array-Processing Language

| Oper. | Type                      | Definition                                                                 |
|-------|---------------------------|-----------------------------------------------------------------------------|
| diff  | (Double⇒Double) ⇒ Double⇒Double | \[
\text{fun } f \ x \rightarrow D[f] (x, 1)
\] |
| grad  | (Vector⇒Double) ⇒ Vector⇒VectorD | \[
\text{build (length } v \text{) (fun } i \rightarrow (D[f] (vectorZip } v \text{ (vectorHot (length } v \text{) } i))
\] |
| jacob | (Vector⇒Vector) ⇒ Vector⇒MatrixD | \[
\text{D}[f] \text{ (vectorZip } v \text{ (vectorHot (length } v \text{) } i))
\] |

Fig. 5. High-Level Differentiation API for \( \tilde{F} \).

If the independent variable has a scalar type, \texttt{deriv} returns the applied function (cf. lines 9-11). However, if the independent variable has a vector type, \texttt{deriv} constructs a vector with the same number of elements as the independent variable. For computing the \( r_i \)th element of the result vector, the corresponding input vector is a one-hot encoding with a single one at the \( r_i \)th position (cf. lines 12 and 39). The situation is similar for an independent variable with a matrix type; the corresponding one-hot encoding matrix has a single one at the \( r_i \) row and \( c_i \)th column (cf. lines 14 and 41). Note that the two variables \( r_i \) and \( c_i \) are treated specially and are distinguished variables.

**Example 2.** Let us assume that we would like to compute the derivative of a program computing the cosine function with respect to its input:

\[
\cos(a)
\]

The derivative of this program at point \( a \) is represented as follows:

\[
\text{snd (deriv (cos a) a)}
\]

This expression is transformed into the following expression after expanding the \texttt{deriv} macro:

\[
\text{snd ((}D[\text{fun } a \rightarrow \cos(a)]) \ (a, 1))
\]

Furthermore, \( \tilde{D} \) provides three additional differentiation constructs, inspired by AD tools such as DiffSharp [7]: 1) \texttt{diff} computes the derivative a function, from a real number to a real number, with respect to its input, 2) \texttt{grad} computes the gradient of a function, from a vector of real numbers to a real number, with respect to its input vector, and 3) \texttt{jacob} computes the Jacobian matrix of a vector-valued function, a function from a vector of real numbers to a vector of real numbers, with respect to its input vector. Figure 5 demonstrates how these high-level differentiation constructs are defined in terms of the source-to-source AD transformation construct \( D \).

**Example 2 (Continued).** For the previous example, if we would like to use the \texttt{diff} construct, first we have to define the following function:

\[
g = \text{fun } x \rightarrow \cos(x)
\]

The derivative of this function at point \( a \) is represented as follows:

\[
\text{snd ((diff } g \text{) a)}
\]

which is expanded to the following program:

\[
\text{snd (}D[g] \ (a, 1))
\]
Algorithm 1 A pseudo-code implementation of the `deriv` construct.

1: // Returns an expression including both the original and the derivative computation.
2: function DERIV(e, x)
3:   args ← ∅
4:   f ← e
5:   for all v ← FREEVARS(e) do
6:     f ← fun v → f
7:     args ← args ∪ DUAL(v, if(v = x) then ONEHOT(v) else ZERO(v))
8:   df ← (∇[f]) args
9:   if TYPE(x) = Double then
10:     return df
11: else if TYPE(x) = Vector then
12:     return build (length x) (fun ri → df)
13: else if TYPE(x) = Matrix then
14:     return build (matrixRows x) (fun ri → build (matrixCols x) (fun ci → df))
15: end function

16: // Returns the dual number encoding of the two input expressions.
17: function DUAL(e₁, e₂)
18:   if TYPE(e₁) = Double then
19:     return (e₁, e₂)
20: else if TYPE(e₁) = Vector then
21:     return vectorZip e₁ e₂
22: else if TYPE(e₁) = Matrix then
23:     return matrixZip e₁ e₂
24: end function

25: // Returns a zero scalar, vector, or matrix expression based on the type of input.
26: function ZERO(e)
27:   if TYPE(e) = Double then
28:     return 0
29: else if TYPE(e) = Vector then
30:     return vectorZeros (length e)
31: else if TYPE(e) = Matrix then
32:     return matrixZeros (matrixRows e) (matrixCols e)
33: end function

34: // Returns a one-hot encoding scalar, vector, or matrix expression.
35: function ONEHOT(e)
36:   if TYPE(e) = Double then
37:     return 1
38: else if TYPE(e) = Vector then
39:     return vectorHot (length e) ri
40: else if TYPE(e) = Matrix then
41:     return matrixHot (matrixRows e) (matrixCols e) ri ci
42: end function
Table 2 summarizes different matrix derivatives, and how they can be computed using our high-level API. Note that the definition of $vdiff$ and $mdiff$ is similar to $diff$, and the definition of $mgrad$ is similar to $grad$ and $jacob$ (cf. Figure 5). Note that the deriv construct subsumes all these operators.

One key advantage of defining different matrix derivatives in terms of automatic differentiation is that one no longer needs to define the matrix calculus derivative rules for all different combinations shown in Table 2. Instead these rules can be deduced automatically from the automatic differentiation rules defined for scalar values. Moreover, even the algebraic identities for matrix derivative can be deduced by using the simplification rules presented in Section 4.

Next, we present the source code transformation required for applying automatic differentiation rules.

### 3.2 Source-to-Source Automatic Differentiation

dAR relies on source-to-source translation for implementing forward-mode automatic differentiation. Each expression is converted into an expression containing both the original computation, together with the derivative computation, a.k.a. the dual number technique. The scalar expressions are transformed into a pair of values, the original computation and the derivative computation. The vector expressions are transformed into vectors containing tuple expressions, instead of scalar expressions. The situation is similar for higher-rank tensors such as matrices.

The rules for automatic differentiation are demonstrated in Figure 6. $\mathcal{D}[e]$ specifies the AD translation for expression $e$. A variable $y$ is translated as $\tilde{y}$, emphasizing that the translated variable keeps the derivative part as well (D-Abs, D-Var, and D-Let). $\mathcal{V}[e]$ is a shorthand for extracting the original computation from the translated term $\mathcal{D}[e]$, while $\mathcal{T}[e]$ is a shorthand for accessing the derivative part. In the case of scalar expressions, $\mathcal{V}[e]$ and $\mathcal{T}[e]$ are equivalent to accessing the first and the second element of the result dual number, respectively (D-NumV and D-NumT).

Constructing an array is differentiated as an array with the same size, however, the way that each element of the array is constructed is differentiated (D-Build). Differentiating an iteration results in an iteration with the same number of iterations, and with the initial state and the next state function both differentiated (D-IFold). The differentiation of the length and indexing an array, is the same as the length and indexing the differentiated array, respectively (D-Length and D-Get).

Differentiating a pair of elements results in the pair of differentiated elements (D-Pair). Similarly, differentiating the projection of a pair, is the projection of the differentiated pair (D-Fst, D-Snd). For other scalar-valued functions, the differentiation rules are similar to the corresponding rules in mathematics.
Example 2 (Continued). In the previous example, based on the automatic differentiation rules, the differentiated program would be as follows:

\[
\tilde{g} = \text{fun } \tilde{x} \rightarrow -\text{snd } (\tilde{x}) \times \sin(\text{fst } (\tilde{x}))
\]

Based on the definition of the \texttt{diff} construct, we have to use the AD version of the function (i.e., \(\tilde{g}\)) and assign 1 to the derivative part of the input. So the value of \(\cos'\) for the input \(a\) is computed as follows:

\[
\text{snd } ((\text{diff } \tilde{g}) \ a) \ \leadsto \ \text{snd } (\mathcal{D}[\tilde{g}] (a, 1)) \ \leadsto \ \text{snd } (\tilde{g} (a, 1)) \ \leadsto \\
-\text{snd } ((a, 1)) \times \sin(\text{fst } ((a, 1))) \ \leadsto \ -1 \times \sin(a) \ \leadsto \ -\sin(a)
\]

Similarly, we can compute the partial derivatives of a given function, by setting the desired derivative part to one, and the rest of derivatives to zero. This process is illustrated in the next example.

Example 3. Assume that we would like to compute the partial derivative of the expression \(a \times b\) with respect to \(a\), which is represented as follows in \(\tilde{\mathcal{F}}\):

\[
\text{snd } (\text{deriv } (a \times b) \ a)
\]

This expression is expanded as follows:

\[
\text{snd } (\mathcal{D}[\text{fun } \tilde{a} \rightarrow \tilde{a} \times \tilde{b}] (a, 1) (b, 0))
\]

Note that the derivative part of the second input is set to 0. Similar to the previous example, the result is as follows:

\[
\text{snd } ((\text{fun } \tilde{a} \rightarrow (\text{fst } (\tilde{a})*\text{fst } (\tilde{b})) + \text{snd } (\tilde{a})*\text{fst } (\tilde{b}))) (a, 1) (b, 0))
\]

which is evaluated as follows:

\[
\text{snd } ((a \times b, 1 \times b + a \times 0)) \ \leadsto \ 1 \times b + a \times 0 \ \leadsto \ b
\]

It is important to note that \(d\tilde{\mathcal{F}}\) performs many of the evaluation steps shown for the previous examples during compilation time, i.e., \(d\tilde{\mathcal{F}}\) performs partial evaluation.

3.3 Perturbation Confusion and Nested Differentiation

In several problems such as computing the Hessian matrix, one requires to compute the differentiation of a differentiated program. In such cases, one should be careful on dealing with tangent parts. We demonstrate this problem in the next example.

Example. Consider the following expression:

\[
\frac{\partial x}{\partial x} \frac{\partial x+y}{\partial y}
\]

This expression should be evaluated to 1 at every point. However, an AD tool can mistakenly evaluate this expression to 2. This is because of confusing the tangent part (perturbation) of the free variable \(x\) with the tangent of the variable \(y\), while computing the inner derivative. This is known as the perturbation confusion problem in the AD literature.

We show how \(d\tilde{\mathcal{F}}\) avoids this problem by using the \texttt{deriv} macro. This expression is implemented as follows in the \(\tilde{\mathcal{F}}\) language:
Efﬁcient Differentiable Programming in a Functional Array-Processing Language

\[
(D-App) \quad D[e_0 \ e_1] = (D[e_0]) (D[e_1])
\]

\[
(D-Abs) \quad D[\text{fun } x \rightarrow e] = \text{fun } \bar{x} \rightarrow D[e]
\]

\[
(D-Var) \quad D[y] = \bar{y}
\]

\[
(D-Let) \quad D[\text{let } x = e_1 \text{ in } e_2] = \text{let } \bar{x} = D[e_1] \text{ in } D[e_2]
\]

\[
(D-If) \quad D[\text{if } e_1 \text{ then } e_2 \text{ else } e_3] = \text{if } (\text{fst } D[e_1]) \text{ then } D[e_2] \text{ else } D[e_3]
\]

\[
(D-Build) \quad D[\text{build } e_0 \ e_1] = \text{build } (\text{fst } D[e_0]) (\text{fun } i \rightarrow (D[e_1]) (i, 0))
\]

\[
(D-IFold) \quad D[\text{ifold } e_0 \ e_1 \ e_2] = \text{ifold } (\text{fun } x \rightarrow (D[e_0]) x (i, 0)) D[e_1] (\text{fst } D[e_2])
\]

\[
(D-Get) \quad D[e_0[e_1]] = (D[e_0]) [f \text{st } D[e_1]]
\]

\[
(D-Length) \quad D[\text{length } e_0] = \text{length } D[e_0], 0
\]

\[
(D-Pair) \quad D[(e_0, e_1)] = (D[e_0], D[e_1])
\]

\[
(D-Fst) \quad D[\text{fst } e_0] = \text{fst } (D[e_0])
\]

\[
(D-Snd) \quad D[\text{snd } e_0] = \text{snd } (D[e_0])
\]

\[
(D-NumV) \quad e: \text{Num} \vdash V[e] = \text{fst } D[e]
\]

\[
(D-NumT) \quad e: \text{Num} \vdash T[e] = \text{snd } D[e]
\]

\[
(D-Neg) \quad D[-e_1] = (-V[e_1], -T[e_1])
\]

\[
(D-Add) \quad D[e_1 + e_2] = (V[e_1]+V[e_2], T[e_1]+T[e_2])
\]

\[
(D-Mult) \quad D[e_1 \ast e_2] = (V[e_1]*V[e_2], T[e_1]*T[e_2] + V[e_1]*T[e_2])
\]

\[
(D-Div) \quad D[e_1 / e_2] = (V[e_1]/V[e_2],
\quad (T[e_1]*V[e_2] - V[e_1]*T[e_2]) / (V[e_2]**2))
\]

\[
(D-Pow) \quad D[e_1 ** e_2] = (V[e_1]**V[e_2], (V[e_2]*T[e_1]) / V[e_1] +
\quad \log(V[e_1])*T[e_2]) * (V[e_1]**V[e_2])
\]

\[
(D-Sin) \quad D[\sin(e_1)] = (\sin(V[e_1]), T[e_1] * \cos(V[e_1]))
\]

\[
(D-Cos) \quad D[\cos(e_1)] = (\cos(V[e_1]), -T[e_1] * \sin(V[e_1]))
\]

\[
(D-Tan) \quad D[\tan(e_1)] = (\tan(V[e_1]), T[e_1] / (\cos(V[e_1]) ** 2))
\]

\[
(D-Log) \quad D[\log(e_1)] = (\log(V[e_1]), T[e_1] / V[e_1])
\]

\[
(D-Exp) \quad D[\exp(e_1)] = (\exp(V[e_1]), T[e_1] * \exp(V[e_1]))
\]

\[
(DT-Fun) \quad D_T[T_1 \Rightarrow T_2] = D_T[T_1] \Rightarrow D_T[T_2]
\]

\[
(DT-Exp) \quad D_T[\text{Num}] = \text{Num} \times \text{Num}
\]

\[
(DT-Arr) \quad D_T[\text{Array<M>}] = \text{Array}<D_T[M]>
\]

\[
(DT-Pair) \quad D_T[M_1 \times M_2] = D_T[M_1] \times D_T[M_2]
\]

Fig. 6. Automatic Differentiation Rules for \( \bar{F} \) Expressions.

\[
\begin{align*}
\text{fun } x \ y \rightarrow \\
\text{snd (}
\text{deriv (x * (snd (}
\text{deriv (x + y) y}
\text{))) x}
\end{align*}
\]

After expanding the inner \texttt{deriv} macro, the following expression is derived:
A. Shaikhha et al.

\[
\text{fun } x \ y \rightarrow \\
\quad \text{snd (} \\
\quad \quad \text{deriv } (x * (\text{snd (} \\
\quad \quad \quad (\text{fun } \bar{x} \ \bar{y} \rightarrow (\text{fst } (\bar{x}) + \text{fst } (\bar{y}), \text{snd } (\bar{x}) + \text{snd } (\bar{y}))) (x, 0) (y, 1) \\
\quad \quad ))) x \\
\quad )
\]

After partially evaluating the inner expression we have:

\[
\text{fun } x \ y \rightarrow \\
\quad \text{snd (} \\
\quad \quad \text{deriv } x \ x \\
\quad )
\]

Expanding this \texttt{deriv} macro results in the following expression:

\[
\text{fun } x \ y \rightarrow \\
\quad \text{snd (} \\
\quad \quad (\text{fun } \bar{x} \rightarrow \bar{x}) (x, 1) \\
\quad )
\]

This expression equivalent to the following expression after partial evaluation:

\[
\text{fun } x \ y \rightarrow \\
\quad 1
\]

Correctly handling the perturbation confusion problem is an important feature, enabling \(\text{d}\tilde{F}\) to efficiently handle nested differentiation constructs such as computing the Hessian matrix. We plan to investigate the support for the Hessian matrix for the future.

Next, we give more details on the optimizations and simplifications offered by \(\text{d}\tilde{F}\).

4 EFFICIENT DIFFERENTIATION

In this section, we show how \(\text{d}\tilde{F}\) achieves efficient differentiable programming. First, we show several transformation rules applicable on \(\tilde{F}\) expressions. Then, we show how we generate C code from \(\tilde{F}\) expressions for a more efficient memory management.

4.1 Transformation Rules

There are various algebraic identities that one can define for \(\tilde{F}\). Based on these identities, differentiated programs can be heavily optimized. Figure 7 shows a set of optimizations defined for \(\tilde{F}\).

There are various optimizations defined for scalar operations based on the ring structure of addition and multiplication, which are shown in Figure 7a. Note that other ring-based algebraic identities, such as associativity and commutativity, do not appear directly in the list of rules that \(\text{d}\tilde{F}\) applies. This is because they do not necessarily improve the performance, unless they are combined with other rewrite rules.

As \(\tilde{F}\) is based on \(\lambda\)-calculus, all partial evaluation rules for this calculus come for free. Furthermore, the optimizations defined in the literature for let-binding can also be used. Finally, partial evaluation rules for conditionals are also available. Figure 7b shows this set of rules.
Efficient Differentiable Programming in a Functional Array-Processing Language

\[
\begin{align*}
e + 0 &= 0 + e 
\Rightarrow e \\
e \cdot 1 &= 1 \cdot e 
\Rightarrow e \\
e \cdot 0 &= 0 \cdot e 
\Rightarrow 0 \\
e + -e &= e - e 
\Rightarrow 0 \\
e_0 \cdot e_1 + e_0 \cdot e_2 &\Rightarrow e_0 \cdot (e_1 + e_2)
\end{align*}
\]

(a) Ring-Structure Rules

\[
\begin{align*}
\text{(fun } x \rightarrow e_0) e_1 &\Rightarrow e_0 \cdot [x \mapsto e_1] \\
\text{let } x = e_0 \text{ in } e_1 &\Rightarrow e_1 \cdot [x \mapsto e_0] \\
\text{let } x = e &\Rightarrow \text{let } y = e_0 \text{ in } e_1 \Rightarrow \text{let } x = e_1 \\
f(\text{let } x = e_0 \text{ in } e_1) &\Rightarrow \text{let } x = e_0 \text{ in } f(e_1)
\end{align*}
\]

(b) \(\lambda\)-Calculus Rules

\[
\begin{align*}
\text{build } e_0 e_1[e_2] &\Rightarrow e_1 e_2 \\
\text{length( build } e_0 e_1) &\Rightarrow e_1 \\
\text{fst } (e_0, e_1) &\Rightarrow e_0 \\
\text{snd } (e_0, e_1) &\Rightarrow e_1
\end{align*}
\]

(c) Fusion Rules

\[
\begin{align*}
\text{ifold } f z 0 &\Rightarrow z \\
\text{ifold } (\text{fun } a \rightarrow a) z n &\Rightarrow z \\
\text{ifold } f z n &\Rightarrow \text{ifold (fun } a \rightarrow f a (i+1)) (f z 0) (n - 1) \\
\text{ifold } (\text{fun } a \rightarrow \text{if}(i = j) \text{ then } f a i else a) z n &\Rightarrow f z j
\end{align*}
\]

(d) Tuple Partial Evaluation Rules

\[
\begin{align*}
\text{if true then } e_1 else e_2 &\Rightarrow e_1 \\
\text{if false then } e_1 else e_2 &\Rightarrow e_2 \\
\text{if } e_0 then e_1 else e_1 &\Rightarrow e_1 \\
f(\text{if } e_0 \text{ then } e_1 \text{ else } e_2) &\Rightarrow \text{if } e_0 \text{ then } f(e_1) \text{ else } f(e_2) \\
\text{if } e_0 \text{ then } e_1 else e_2 &\Rightarrow \text{if } e_0 \text{ then } e_1[e_0 \mapsto \text{true}] else e_2[e_0 \mapsto \text{false}]
\end{align*}
\]

(e) Iteration Rules

\[
\begin{align*}
\text{ifold } (\text{fun } a \rightarrow (f (\text{fst } a) i, g (\text{snd } a) i)) (z_1, z_2) n &\Rightarrow \text{ifold } f z 1 n, \text{ifold } g z 2 n
\end{align*}
\]

(f) Conditional Rules

\[
\begin{align*}
\text{ifold } (\text{fun } a \rightarrow (f (\text{fst } a) i, g (\text{snd } a) i)) (z_1, z_2) n &\Rightarrow \text{ifold } f z 1 n, \text{ifold } g z 2 n)
\end{align*}
\]

(g) Loop Fission

Fig. 7. Optimizations for \(\tilde{F}\).

As the vector constructs of \(\tilde{F}\) are based on pull arrays, one can use the pull-array fusion rules for removing unnecessary intermediate vectors and matrices. The two fusion rules for pull-arrays are shown in Figure 7c.

In addition, many intermediate tuples resulting from the dual number technique of AD can be removed by using partial evaluation. Figure 7d shows the partial evaluation rules for removing the intermediate tuples which are followed by a projection.

Partially evaluating the tuples across the boundary of a loop requires a sophisticated analysis of the body of the loop. To simplify this task, we perform loop fission for the loops that return a tuple of values. This is possible only when different elements of the tuple are computed independently in different iterations of the loop. Figure 7g shows how loop fission turns an iteration creating a pair of elements into a pair of two iterations constructing independently the elements of that pair. After performing this optimization, if we are interested only in a particular element of the result tuple, other loops corresponding to irrelevant elements are removed by partial evaluation.

Based on these rewrite rules, \(d\tilde{F}\) derives well-known matrix calculus rules, without requiring to add a rewrite rule in the level of matrices (i.e., \(\tilde{M}\)). However, as we will see, the order in which these rewrite rules should be applied can become tricky and for the moment are
defined manually in \(d\mathcal{F}\). We leave an automatic way of inferring a good sequence of rewrite rules for the future work.

The next example, shows how \(d\mathcal{F}\) can derive a well-known matrix identity by using a sequence of transformation rules defined in this section.

**Example 4.** Based on matrix calculus derivative rules, it is known that \(\frac{\partial v_1 \cdot v_2}{\partial v_1} = v_2\), where \(\cdot\) is the vector dot product operator. We would like to show how \(d\mathcal{F}\) can deduce the same algebraic identity. The differentiation of dot product of two vectors is represented as follows:

\[
\text{fun } v_1 v_2 \rightarrow \\
\text{vectorMap (deriv (vectorDot v1 v2) v1) snd}
\]

This expression is expanded as follows:

\[
\text{fun } v_1 v_2 \rightarrow \\
\text{vectorMap (} \\
\text{build (length v1) (fun i ->} \\
\text{D[fun v1 v2 -> vectorDot v1 v2] (vectorZip v1 (vectorHot (length v1) i))} \\
\text{vectorZip v2 (vectorZeros (length v2)))}) \text{snd}
\]

After inlining the definition of \text{vectorMap} (cf. Figure 4) and applying the fusion rule (cf. Figure 7c), the following program is produced:

\[
\text{fun } v_1 v_2 \rightarrow \\
\text{build (length v1) (fun i ->} \\
\text{snd (D[fun v1 v2 -> vectorDot v1 v2] (vectorZip v1 (vectorHot (length v1) i))} \\
\text{vectorZip v2 (vectorZeros (length v2)))})
\]

After inlining the definition of \text{vectorDot, vectorZip, vectorHot, and vectorZeros}, and again applying the fusion rule, we have:

\[
\text{fun } v_1 v_2 \rightarrow \\
\text{build (length v1) (fun i ->} \\
\text{snd (D[fun v1 v2 -> ifold (fun s j -> s + v1[j] \cdot v2[j]) 0 (length v1)] (build (length v1) (fun j -> (v1[j], if(i=j) then 1 else 0)))} \\
\text{build (length v2) (fun j -> (v2[j], 0))))}
\]

After applying AD transformation rules (cf. Figure 6), and partial evaluation rules (cf. Figure 7) the following program is derived:

\[
\text{fun } v_1 v_2 \rightarrow \\
\text{build (length v1) (fun i ->} \\
\text{snd (fun v1 v2 -> iifold (fun s j ->} \\
\text{( (fst s) + (fst v1[j]) \cdot (fst v2[j]),} \\
\text{(snd s) + (fst v1[j]) \cdot (snd v2[j]) + (snd v1[j]) \cdot (fst v2[j]) )} \\
\text{)} (0, 0) (length v1)) (build (length v1) (fun j -> (v1[j], if(i=j) then 1 else 0)))} \\
\text{build (length v2) (fun j -> (v2[j], 0))))}
\]
Efficient Differentiable Programming in a Functional Array-Processing Language

After further applying $\beta$-reduction (cf. Figure 7b), tuple partial evaluation (cf. Figure 7b), and loop fusion the following program is generated:

```plaintext
fun v1 v2 ->
    build (length v1) (fun i ->
        snd (ifold (fun s j ->
            ( (fst s) + v1[j] * v2[j] ,
              (snd s) + v1[j] * 0 + (if (i=j) then 1 else 0) * v2[j] )
        ) (0, 0) (length v1))
    )
```

Now we apply loop fission (cf. Figure 7g), conditional rules (cf. Figure 7f), and several other simplification rules:

```plaintext
fun v1 v2 ->
    build (length v1) (fun i ->
        snd (ifold (fun s j -> s + v1[j] * v2[j]) 0 (length v1) ,
            ifold (fun s j -> if (i=j) then s + v2[j] else s) 0 (length v1))
    )
```

Note that applying the loop fission rule, does not necessarily improve the performance; it is only after performing tuple partial evaluation rules that the iteration responsible for the original computation is removed and the performance is improved. Thus, the strategy for applying rewrite rules can become tricky, and for this example, we manually specify the sequence of transformations that should be applied. After applying the partial evaluation rule, the following program is derived:

```plaintext
fun v1 v2 ->
    build (length v1) (fun i ->
        ifold (fun s j ->
            if (i = j) then
                (s + v2[j])
            else
                s)
        0 (length v1)))
```

By using the optimization that turns single access iterations into a single statement (cf. Figure 7e), $d\bar{F}$ produces the following program:

```plaintext
fun v1 v2 ->
    build (length v1) (fun i ->
        v2[i])
```

This program is equivalent to $v2$ if the size of the two input vectors are the same (i.e., $\text{length } v1 = \text{length } v2$). Otherwise, the input program is ill-formed.

Next, we show the power of $d\bar{F}$ in deriving a matrix calculus identity for gradient of matrices.

**Example 5.** By using the same set of optimizations, $d\bar{F}$ can deduce the identity $\frac{\partial \text{Tr}(M)}{\partial M} = I$.

First, we start from the representation of this gradient in $\bar{F}$:

```plaintext
fun m ->
    build (length m) (fun i ->
        build (length m[0]) (fun j ->
            snd (D[\text{matrixTrace}] (matrixZip m (matrixHot (length m) (length m[0]) i j))))
    )
```

\[\triangle \]

Vol. 1, No. 1, Article . Publication date: April 2018.
After applying the AD transformations and the optimizations presented in this section, the following program is produced:

```haskell
fun m ->
  build (length m) (fun i ->
    build (length m[0]) (fun j ->
      if (j = i) then 1 else 0))
```

If the rows and columns of the input matrix are equal, this program represents the identity matrix with the same dimensions as the input matrix.

Similarly, $\tilde{d}$ automatically discovers the following identity if $A$ is independent of $M$:

$$\frac{\partial \text{tr}(MA)}{\partial M} = A^T.$$ Now we return to the example shown in the beginning of this paper.

**Example 1 (Continued).** If we have a matrix $M$ and two vectors $u$ and $v$ (which are represented as row matrices and are independent of $M$), using matrix calculus one can prove that

$$\frac{\partial (uMv^T)}{\partial M} = u^T v.$$ First, we start by a partially inlined representation of this program in $\tilde{F}$:

```haskell
let f = fun u M v ->
  let m =
    matrixMult
      (build 1 (fun i -> u))
      (matrixMult M
        (matrixTranspose (build 1 (fun i -> v))))
    m[0][0]
  fun u M v ->
    (build (length M) (fun i ->
      (build (length M[0]) (fun j ->
        snd (D[f]
          (vectorZip v (vectorZeros (length v))))
          (matrixZip M (matrixHot (length M) (length M[0]) i j))
          (vectorZip v (vectorZeros (length v))))))))))
```

Note that the function $f$ is returning the only scalar element of the 1-by-1 matrix $uMv^T$. After performing loop fusion, loop fission and partial evaluation the following program is derived:

```haskell
fun u M v ->
  build (length M) (fun i ->
    build (length M[0]) (fun j ->
      u[i] * v[j]))
```

This program is equivalent to $u^T v$ if the input program is well formed, i.e., the number of rows and columns of $M$ are the same as the length of $u$ and $v$, respectively.
4.2 Code Generation

After applying the optimizations mentioned in the previous section, one can further improve the efficiency by generating programs in a low-level language with manual memory management. This way, the overhead of garbage collection can be removed. Furthermore, by using stack-discipline memory management techniques such as Destination-Passing Style (DPS) [44], one can benefit from efficient bump memory allocation instead of using the expensive `malloc` and `free` calls.

Example 1 (Continued). The generated C code for the optimized differentiated program is as follows:

```c
matrix uMv_d(storage s, vector u, matrix M, vector v) {
    matrix res = (matrix)s;
    for (int r = 0; r < M->rows; r++) {
        for (int c = 0; c < M->cols; c++) {
            res->elems[r][c] = u->elems[r] * v->elems[c];
        }
    }
    return res;
}
```

The parameter `s` is the storage area allocated for storing the result matrix.

Up to now, we have only seen the cases where only the derivative part of the program was of interest. If we are interested in the original part of the program as well (e.g., the intermediate vectors cannot be fused), we need to store both the original and derivative parts. In such cases, the differentiated vectors, which are represented as arrays of tuples, can be transformed into a more efficient data layout. The well-known array of structs (AoS) to struct of arrays (SoA) transformation represents differentiated vectors as a tuple of two numeric arrays. Further partial evaluation can remove the unnecessary decoupled numeric arrays.

5 EXPERIMENTAL RESULTS

In this section, we show how $\tilde{dF}$ performs in practice. We show the performance of the differentiated code for two real-world machine learning and computer vision applications.

Experimental Setup. We have performed the experiments using an iMac machine equipped with an Intel Core i5 CPU running at 2.7GHz, 32GB of DDR3 RAM at 1333Mhz. The operating system is OS X 10.13.1. We use CLang 900.0.39.2 for compiling the generated C code, and Python 2.7.12 for running the Python code.

Micro Benchmarks which consist of the following vector expressions: 1) gradient of dot product of two vectors with respect to the first vector (which is a Jacobian matrix with a single row), 2) gradient of the maximum value of a vector with respect to the input vector (which is a Jacobian matrix with a single row), 3) gradient of addition of two vectors with respect to the first vector (which is a Jacobian matrix), and 4) gradient of the multiplication of a vector with a scalar value with respect to the scalar value (which is a Jacobian matrix with a single column).

Figure 8 shows the performance results for the mentioned micro benchmarks for $\tilde{dF}$ and both forward and reverse-mode of Tapenade. In all cases, $\tilde{dF}$ outperforms or performs as good as both forward and reverse-mode of Tapenade. The performance is improved further when the generated C code uses Destination-Passing Style (DPS) [44] for stack-discipline memory management.
As in the first two cases the Jacobian matrix is a row vector, reverse-mode AD computes the whole Jacobian matrix in a single backward pass. However, forward-mode AD needs to iterate over each column to compute the corresponding derivative value. For the case of the addition of two vectors, as the Jacobian matrix is a square matrix, reverse-mode AD and forward-mode AD show comparable performance. Finally, for the last case, as the Jacobian matrix is a column vector, the forward mode AD computes the whole Jacobian matrix in a single forward pass. However, the reverse mode AD requires traversing over each row to compute the corresponding partial derivative values.

Non-Negative Matrix Factorization (NNMF) is a useful tool which has many applications in various fields ranging from document clustering, recommendation systems, signal processing, to computer vision. For instance, in [32], the authors study the NNMF of Web dyadic data represented as the matrix $A$. Dyadic data contains rich information about the interactions between the two participating sets. It is useful for a broad range of practical applications including Web search, Internet monetization, and social media content [32]. For example the (query, clicked URL) data is used in query clustering [28], query suggestions [5] and improving search relevance [3]. Matrix factorization is a commonly used approach to understanding the latent structure of the observed matrix for various applications [9, 47].
a probabilistic NNMF framework for a variety of Web dyadic data that conforms to different probabilistic distributions. For instance, an Exponential distribution is used to model Web lifetime dyadic data, e.g., user dwell time, and similarly the Poisson distribution is used to model count dyadic data, e.g., click counts.

The iterative algorithm to find $W$ and $H$ depends on the form of the assumed underlying distribution. In particular the update formula for gradient descent are derived by computing the gradient of the negative log of the likelihood function. For example, the negative log of the exponential distribution is represented as follows:

$$D(A||\tilde{A}) = \sum_{i,j} \left( \log(\tilde{A}_{i,j}) + \frac{A_{i,j}}{\tilde{A}_{i,j}} \right), \quad \tilde{A} = WH$$

The update formulas are derived manually, and for each new distribution it is the responsibility of the user to undertake the error prone and laborious task of deriving, optimizing, and implementing the update rules. d\textbar\textbar automatically derives the gradient of the negative log of the likelihood function for the exponential distribution. After performing optimizations, d\textbar\textbar produces an expression which is equivalent to the following update formula, which is manually derived by hand in [32]:

$$\frac{\partial D}{\partial H} = W^T \left( \frac{1}{WH} - \frac{A}{(WH)^2} \right)$$

Figure 9 shows the performance results of executing the derived update rule on Tapenade, Theano, and d\textbar\textbar. For all the experiments, we consider factorizing the matrix $A$ into two vectors $W$ and $H$ (represented as $u$ and $v^T$, respectively). To have a fair comparison between Tapenade and d\textbar\textbar, we have provided both the fused and unfused versions of the likelihood function. We observe a 2x speed up for the forward mode, and a 5x speed up for the reverse mode, when comparing the fused version with the unfused version. Comparing the fused version of Tapenade and d\textbar\textbar, we observe that the reverse-mode AD of Tapenade behaves similarly to d\textbar\textbar. This shows that d\textbar\textbar successfully generates efficient code for this case, which is an ideal case for the reverse-mode AD (the loss function is a scalar valued function, which should compute the gradient with respect to all elements of the input vector). Finally, as the dimension of the vectors increases, Theano converges to the same performance as d\textbar\textbar and reverse-mode AD of Tapenade. This is thanks to the fact that the overhead of invoking C functions from Python becomes negligible as the size of the vector increases.
**The Gaussian Mixture Model (GMM)** is a statistical method used for various machine learning tasks such as unsupervised and semi-supervised learning, as well as computer vision applications such as image background modelling and image denoising.

Here we focus on computing the gradient of one of function used in GMM: the Log-Sum-Exp (LSE) of a vector is useful in various machine learning algorithms such as GMM [25, 37]. Intuitively, if the multiplication operation in the linear domain is transformed into addition in the log domain, the addition operation is transformed into LSE in the log domain. This expression is computed as follows.

\[
\text{LSE}(x_1, \ldots, x_n) = x_{\max} + \log\left(\sum_{i=1}^{n} e^{x_i - x_{\max}}\right)
\]

Figure 10 shows the performance results for the gradient of this function with respect to its input vector. Applying fusion improves the performance of the differentiated programs by 25%. Comparing the fused versions of the programs, \(\tilde{\text{df}}\) outperforms the forward-mode AD of Tapenade from 2 to 4 orders of magnitude. This gap increases quadratically with the size of the input vector. However, \(\tilde{\text{df}}\) shows a similar performance to the fused reverse-mode AD of Tapenade.

**Bundle Adjustment** [2, 53, 56] is a computer vision problem, where the goal is to optimize several parameters in order to have an accurate estimate of the projection of a 3D point by a camera. This is achieved by minimizing an objective function representing the reprojection error.

For the experiments, we compute the Jacobian matrix of the Project function in Bundle Adjustment. For a 3D point \(X \in \mathbb{R}^3\) and a camera with rotation parameter \(r \in \mathbb{R}^3\), center position \(C \in \mathbb{R}^3\), focal index \(f \in \mathbb{R}\), principal point \(x_0 \in \mathbb{R}^2\), and radical distortion \(k \in \mathbb{R}^2\), the Project function is computes the projected point as follows:

\[
\text{project}(r, C, f, x_0, k, X) = \text{distort}(k, p2e(\text{rodrigues}(r, X - C))) f + x_0
\]
\[
\text{distort}(k, x) = x(1 + k_1||x||^2 + k_2||x||^4)
\]
\[
p2e(X) = X_{1,2}X_3
\]
\[
\text{rodrigues}(r, X) = X\cos\theta + (v \times X)\sin\theta + v(v^TX)(1 - \cos\theta), \theta = ||r||, v = \frac{r}{||r||}
\]

Consider having \(N\) 3D points and one particular camera parameter (an input vector of size \(3N + 11\)), we are interested in computing a Jacobian matrix with \(3N + 11\) rows and \(2N\)
columns. Figure 11 shows the performance results for computing the mentioned Jacobian matrix. As it can be seen \( \bar{dF} \) outperforms both forward and reverse mode of Tapenade. This is mainly thanks to the loop transformations, such as loop-invariant code motion, happening in \( \bar{dF} \).

6 RELATED WORK

Automatic Differentiation. There is a large body of work on automatic differentiation (AD) of imperative programming languages. Tapenade [21] performs AD for a subset of C and Fortran, whereas, ADIFOR [10] performs AD for Fortran programs. Adept [24] and ADIC [36] perform automatic differentiation for C++ by using expression templates. However, as we have seen in our experimental results, an AD tool such as Tapenade misses several optimization opportunities, mainly due to their limited support for loop fusion.

ADiMat [11], ADiGator [55], and Mad [18] perform AD for MATLAB programs, whereas MuPAD [23] computes the derivatives using symbolic differentiation. AutoGrad [33] performs AD for Python programs that use NumPy library for array manipulation, whereas Theano [8] uses symbolic differentiation. Tensorflow [1] performs source-to-source reverse-mode AD, and uses advanced heuristics to solve the memory inefficiencies. ForwardDiff [43] employs vector forward-mode AD [30] for differentiating Julia programs. This system keeps a vector of derivative values in the dual number instead of only a single derivative value. All these systems miss important optimization opportunities such as loop fusion.

DiffSharp [7] is an AD library implemented in F#. This library provides both forward-mode and reverse-mode AD techniques. As DiffSharp is a library implementation of AD (in contrast to \( \bar{dF} \), which implements AD as source-to-source transformation rules), it cannot not support the simplification rules such as loop-invariant code motion, loop fusion, and partial evaluation. Furthermore, \( \bar{dF} \) can efficiently manage memory by generating C code using DPS, whereas DiffSharp should rely on the garbage collection provided by the .NET framework for memory management.

Stalingrad [40] is an optimizing compiler for a dialect of Scheme with a first-class AD operator, with the support for both forward mode and reverse mode of AD. One of the key challenges that Stalingrad addresses is perturbation confusion [45], which occurs for computing the derivative of the functions for which the derivatives are already computed,
or the cases where we need the computation of nested differentiation [39]. We have shown in Section 3.3 how dF̃ resolves the perturbation confusion problem. One key limitation of Stalingrad is the lack of support for variable-size vectors; Stalingrad only supports a statically-known-size list of elements which are unfolded using Scheme macros.

Karczmarczuk [29] presents a Haskell implementation for both forward and reverse mode AD. Elliott [17] improves this work by giving a more elegant implementation for its forward mode AD. These implementations lack the optimizations offered by transformation rules, such as loop fusion.

**Array Languages and Fusion.** There are many array programming languages in the literature, APL [27] being the pioneer among them. There are functional array languages such as Futhark [22] and SAC [20] with support for fusion.

In array languages fusion can be achieved by using functional arrays known as push and pull arrays [4, 13, 52]. A push-array is represented by an effectful function that, given an index and a value, will write the value into the array. A pull-array is represented by the length of the array and a function producing an element for a given index, similar to the build construct in F̃. Similarly, functional programming languages use shortcut deforestation for fusing lists either by pulling the stream of data [14, 51] or pushing them [19].

**Numerical DSLs.** There are many DSLs for numerical workloads. These DSLs can be classified in three categories. The first category consists of mainstream programming languages used by data analysts such as MATLAB and R. These languages offer many toolboxes for performing a wide range of tasks, however, from a performance point of view the focus is only on the efficient implementation of the libraries. The second category consists of DSLs such as Lift [49], Opt [16], Halide [42], Diderot [12], and OptiML [50], which generate parallel code from their high-level programs. The third category is the DSLs which focus on generating efficient machine code for fixed size algebra problems such as Spiral [41] and LGen [46]. These DSLs exploit the memory hierarchy by relying on searching algorithms for making tiling and scheduling decisions. Except the first category, for which automatic differentiation tools exist, the other DSLs do not have any support for automatic differentiation. Moreover, parallel code generation and efficient machine code generation are orthogonal concepts and can be added to dF̃ in the future.

7 OUTLOOK AND CONCLUSIONS

In this paper we have demonstrated how to efficiently compute the derivative of a program. The key idea behind our system is exposing all the constructs used in differentiated programs to the underlying compiler. As a result, the compiler can apply various loop transformations such as loop-invariant code motion and loop fusion for optimizing differentiated programs. We have shown how dF̃ outperforms the existing AD tools on micro benchmarks and real-world machine learning and computer vision applications.

We plan to extend dF̃ with the reverse-mode AD by employing a similar technique to the one proposed by [40]. In addition, as we have seen in our examples, the strategy for applying rewrite rules can become tricky in some cases; there are some rewrite rules (e.g., loop fission) that do not necessarily improve the performance, unless they are combined with other transformation rules. We plan to investigate the use of search strategies for automated rewriting (e.g., using Monte-Carlo tree search [15]).

REFERENCES

[1] Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, et al. 2016. TensorFlow: A System for Large-Scale
Efficient Differentiable Programming in a Functional Array-Processing Language

Machine Learning. In *OSDI*, Vol. 16. 265–283.

[2] Sameer Agarwal, Noah Snavely, Steven M Seitz, and Richard Szeliski. 2010. Bundle adjustment in the large. In *European conference on computer vision*. Springer, 29–42.

[3] Eugene Agichtein, Eric Brill, and Susan Dumais. 2006. Improving Web Search Ranking by Incorporating User Behavior Information. In *SIGIR*.

[4] Johan Anker and Josef Svenningsson. 2013. An EDSL approach to high performance Haskell programming. In *ACM Haskell Symposium*. 1–12.

[5] Ricardo Baeza-Yates, Carlos Hurtado, and Marcelo Mendoza. 2004. Query Recommendation Using Query Logs in Search Engines. In *EDBT*.

[6] Atilim Gunes Baydin, Barak A Pearlmutter, Alexey Andreyevich Radul, and Jeffrey Mark Siskind. 2015. Automatic differentiation in machine learning: a survey. arXiv preprint arXiv:1502.05767 (2015).

[7] Atilim Gunes Baydin, Barak A Pearlmutter, and Jeffrey Mark Siskind. 2015. Diffsharp: Automatic differentiation library. arXiv preprint arXiv:1511.07727 (2015).

[8] James Bergstra, Olivier Breuleux, Frédéric Bastien, Pascal Lamblin, Razvan Pascanu, Guillaume Desjardins, Joseph Turian, David Warde-Farley, and Yoshua Bengio. 2010. Theano: A CPU and GPU math compiler in Python. In *Proc. 9th Python in Science Conf*. 1–7.

[9] Michael W. Berry, Murray Browne, Amy N. Langville, V. Paul Pauca, and Robert J. Plemmons. 2006. Algorithms and applications for approximate nonnegative matrix factorization. In *Computational Statistics and Data Analysis*.

[10] Christian Bischof, Peyvand Khademi, Andrew Mauer, and Alan Carle. 1996. ADIFOR 2.0: Automatic differentiation of Fortran 77 programs. *IEEE Computational Science and Engineering* 3, 3 (1996), 18–32.

[11] Christian H Bischof, HM Bucker, Bruno Lang, Arno Rasch, and Andre Vehreschild. 2002. Combining source transformation and operator overloading techniques to compute derivatives for MATLAB programs. In *Source Code Analysis and Manipulation, 2002. Proceedings. Second IEEE International Workshop on*. IEEE, 65–72.

[12] Charisee Chiw, Gordon Kindlmann, John Reppy, Lamont Samuels, and Nick Seltzer. 2012. Diderot: A Parallel DSL for Image Analysis and Visualization (PLDI ’12). ACM, 111–120.

[13] Koen Claessen, Mary Sheeran, and Bo Joel Svensson. 2012. Expressive Array Constructs in an Embedded GPU Kernel Programming Language (DAMP ’12). ACM, NY, USA, 21–30.

[14] Duncan Coutts, Roman Leschchinskiy, and Don Stewart. [n. d.]. Stream Fusion. From Lists to Streams to Nothing at All (ICFP ’07).

[15] Frédéric De Mesmay, Arpad Rimmel, Yevgen Voronenko, and Markus Püschel. 2009. Bandit-based optimization on graphs with application to library performance tuning. In *Proceedings of the 26th Annual International Conference on Machine Learning*. ACM, 729–736.

[16] Zachary DeVito, Michael Mara, Michael Zollhöfer, Gilbert Bernstein, Jonathan Ragan-Kelley, Christian Theobalt, Pat Hanrahan, Matthew Fisher, and Matthias Nießner. 2016. Opt: A Domain Specific Language for Non-linear Least Squares Optimization in Graphics and Imaging. arXiv preprint arXiv:1604.06525 (2016).

[17] Conal M Elliott. 2009. Beautiful differentiation. In *ACM Sigplan Notices*, Vol. 44. ACM, 191–202.

[18] Shaun A Forth. 2006. An efficient overloaded implementation of forward mode automatic differentiation in MATLAB. *ACM Transactions on Mathematical Software (TOMS)* 32, 2 (2006), 195–222.

[19] Andrew Gill, John Launchbury, and Simon L Peyton Jones. 1993. A short cut to deforestation (FPCA). ACM, 223–232.

[20] Clemens Greckel and Sven-Bodo Scholz. 2006. SAC—A Functional Array Language for Efficient Multi-threaded Execution. *Int. Journal of Parallel Programming* 34, 4 (2006), 383–427.

[21] Laurent Hascoet and Valérie Pascual. 2013. The Tapenade Automatic Differentiation Tool: Principles, Model, and Specification. *ACM Trans. Math. Softw.* 39, 3, Article 20 (May 2013), 43 pages. https://doi.org/10.1145/2450153.2450158

[22] Troels Henriksen, Niels GW Serup, Martin Elsman, Fritz Henglein, and Cosmin E Oancea. 2017. Futhark: purely functional GPU-programming with nested parallelism and in-place array updates. In *Proceedings of the 38th ACM SIGPLAN Conference on Programming Language Design and Implementation*. ACM, 556–571.

[23] Florent Hivert and N Thiéry. 2004. MuPAD-Combinat, an open-source package for research in algebraic combinatorics. *Sém. Lothar. Combin* 51 (2004), 70.

[24] Robin J. Hogan. 2014. Fast Reverse-Mode Automatic Differentiation Using Expression Templates in C++. *ACM Trans. Math. Softw.* 40, 4, Article 26 (July 2014), 16 pages. https://doi.org/10.1145/2560359
Efficient Differentiable Programming in a Functional Array-Processing Language

OpenCL Code. In Proceedings of the 20th ACM SIGPLAN International Conference on Functional Programming (ICFP 2015). ACM, New York, NY, USA, 205–217. https://doi.org/10.1145/2784731.2784754

[50] Arvind Sujeeth, HyoukJoong Lee, Kevin Brown, Tiark Rompf, Hassan Chafi, Michael Wu, Anand Atreya, Martin Odersky, and Kunle Olukotun. 2011. OptiML: An Implicitly Parallel Domain-Specific Language for Machine Learning (ICML ’11). 609–616.

[51] Josef Svenningsson. 2002. Shortcut Fusion for Accumulating Parameters & Zip-like Functions (ICFP ’02). ACM, 124–132.

[52] Bo Joel Svensson and Josef Svenningsson. 2014. Defunctionalizing Push Arrays (FHPC ’14). ACM, NY, USA, 43–52.

[53] Bill Triggs, Philip F McLauchlan, Richard I Hartley, and Andrew W Fitzgibbon. 1999. Bundle adjustment—a modern synthesis. In Inter. workshop on vision algorithms. Springer, 298–372.

[54] Philip Wadler. 1988. Deforestation: Transforming programs to eliminate trees. In ESOP’88. Springer, 344–358.

[55] Matthew J Weinstein and Anil V Rao. 2016. Algorithm: ADiGator, a toolbox for the algorithmic differentiation of mathematical functions in MATLAB using source transformation via operator overloading. ACM Trans. Math. Softw (2016).

[56] Christopher Zach. 2014. Robust bundle adjustment revisited. In European Conference on Computer Vision. Springer, 772–787.