DON’T UNROLL ADJOINT: DIFFERENTIATING SSA-FORM PROGRAMS

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ABSTRACT
This paper presents reverse-mode algorithmic differentiation (AD) based on source code transformation, in particular of the Static Single Assignment (SSA) form used by modern compilers. The approach can support control flow, nesting, mutation, recursion, data structures, higher-order functions, and other language constructs, and the output is given to an existing compiler to produce highly efficient differentiated code. Our implementation is a new AD tool for the Julia language, called Zygote, which presents high-level dynamic semantics while transparently compiling adjoint code under the hood. We discuss the benefits of this approach to both the usability and performance of AD tools.

1 INTRODUCTION
Reverse-mode algorithmic differentiation (AD) (Speelpenning, 1980) is at the heart of recent developments in machine learning (ML) and deep learning (Baydin et al., 2017). ML systems place extreme demands on the tools used to build them; they typically require the highest performance, yet researchers increasingly need the flexibility of a fully differentiable programming language (Innes et al., 2018).

AD systems face a tradeoff between providing an expressive, full-featured programming model and producing optimised programs (Neubig et al., 2017). Current ML frameworks use tracing approaches to record the numerical operations in the program, which is simple to implement but has significant limitations (Section 2.3). Preserving host language semantics (e.g. control flow) requires dynamically building the trace, which adds overhead and precludes many optimisations (Maclaurin et al., 2015). Saving and compiling traces helps performance at the cost of significantly reduced expressiveness (Bergstra et al., 2011). Avoiding tracing via source-to-source techniques resolves this tradeoff to some extent but has previously been cumbersome or supported only limited semantics (Pearlmutter & Siskind, 2008; Hascoet & Pascual, 2013). Saving and compiling traces helps performance at the cost of significantly reduced expressiveness (Bergstra et al., 2011). Avoiding tracing via source-to-source techniques resolves this tradeoff to some extent but has previously been cumbersome or supported only limited semantics (Pearlmutter & Siskind, 2008; Hascoet & Pascual, 2013).

Section 3 describes AD over a Static Single Assignment (SSA) representation of programs in a way that supports control flow, higher-order functions and nested derivatives. The differentiated code can be further fed into a traditional compiler such as LLVM (Lattner & Adve, 2004), which results in an extremely efficient derivative program. Further, it opens up the opportunity for robust traditional compiler techniques to be extended to machine learning, enabling kernel fusion or compilation for accelerators with no artificial limitations on the kinds of models that researchers can express. This combination has not previously been possible in a high-level, general-purpose programming language.

We additionally introduce Zygote, a working implementation of this technique which augments the Julia compiler (Bezanson et al., 2017) and is designed for use with the Flux machine learning library (Innes, 2018). Unlike tools such as Tapenade (Hascoet & Pascual, 2013), which have similar goals, Zygote never exposes source transformations to the user; it is an implementation detail of a familiar gradient(f, x) interface that can naturally express nested derivatives. We discuss Zygote’s interaction with Julia’s programming model and compiler, and the performance characteristics that result from this combination.

2 TAPES & WENGER LISTS
2.1 Notation & Background
Given a target program that outputs a scalar l (typically a loss or objective to be minimised), we write the gradient ∂l/∂x as ∇x. For uniformity we do not specify the derivatives of component functions like sin(x) or a × b directly in the rules of differentiation, but instead treat these as handled via a higher-order differentiation function J (Pearlmutter & Siskind, 2008). Given a function y = f(x1, x2, ...), we write ∇x B, J = J(f, x, y); J returns the usual result y as well as a backpropagator function B. Then ∇x, y = B(∇x); the backpropagators are linear func-
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Table 1. Backpropagators for some simple mathematical functions.

| Function     | Backpropagator |
|--------------|----------------|
| \( y = a + b \) | \((\bar{y}, \bar{y})\) |
| \( y = a \times b \) | \((\bar{y} \times b, y \times a)\) |
| \( y = \sin(x) \) | \(\bar{y} \times \cos(x)\) |
| \( y = \exp(x) \) | \(\bar{y} \times y\) |
| \( y = \log(x) \) | \(\bar{y}/x\) |

This notation has the benefit of treating program subroutines uniformly with mathematical primitives. In the vector case \( \partial y/\partial x \) may be a large Jacobian which we wish to avoid instantiating explicitly. Calling \( J \) with a user-defined \( f \) can generate an appropriate backpropagator for some AD technique (such as the one we describe).

2.2 Differentiating Wengert Lists

Consider the following mathematical function, which may be part of our target program. We assume that \( y \) is further used to calculate \( l \), and that we know \( \partial l/\partial y \).

\[
y = f(a, b) = \frac{a}{a + b^2}
\]

We can rewrite this equivalently by naming each intermediate result.

\[
y_1 = b^2 \\
y_2 = a + y_1 \\
y_3 = \frac{a}{y_2}
\]

This form can be viewed as a limited programming language; it is often referred to as a Wengert list, tape or graph (Bartholomew-Biggs et al., 2000). The Wengert list is easy to differentiate. First wrap all function calls with \( J \) to create a primal version of \( f \).

\[
y_1, B_1 = J(\cdot, b, 2) \\
y_2, B_2 = J(\cdot, a, y_1) \\
y_3, B_3 = J(\cdot, a, y_2)
\]

Given the gradient \( \bar{y}_i \), we can call the backpropagator \( B_i \) to get gradients for the inputs to \( y_i \). Where a variable \( x \) is used multiple times, each corresponding backpropagator produces a contribution to the gradient (the \( \bar{a}_i \), below) which must be summed. This is motivated by the multivariate chain rule given in equation 2.

\[
x = \frac{\partial l}{\partial x} = \frac{\partial l}{\partial y_1} \frac{\partial y_1}{\partial x} + \frac{\partial l}{\partial y_2} \frac{\partial y_2}{\partial x} \quad (2)
\]

\[
x = B_{y_1}(\bar{y}_1) + B_{y_2}(\bar{y}_2) \quad (3)
\]

By applying these steps we can begin with the gradient \( \bar{y} = 1 \) and proceed in reverse over the list to get \( \partial y/\partial a \) and \( \partial y/\partial b \). This can be realised either by interpreting the Wengert expression in reverse, or by explicitly creating an adjoint expression as follows.

\[
\bar{y}_3 = 1 \\
\bar{a}_1, \bar{y}_2 = B_3(\bar{y}_3) \\
\bar{a}_2, \bar{y}_1 = B_2(\bar{y}_2) \\
\bar{a} = \bar{a}_1 + \bar{a}_2 \\
\bar{b} = B_1(\bar{y}_1)
\]

Realising this code as a function, with \( \bar{y}_3 \) as an argument, creates the backpropagator for \( f \). Inlining all function calls yields an efficient symbolic derivative; the \( J \) notation really is just notation.

\[
y_2 = a + b^2 \\
\bar{y}_2 = -\frac{a}{y_2^2} \\
y = \frac{a}{y_2} \\
\bar{a} = \frac{1}{y_2} + \bar{y}_2 \\
\bar{b} = 2b\bar{y}_2
\]

2.3 Tapes in Practice

To see how Wengert lists can be used to differentiate programs, consider a simple implementation of \( x^n \) (for natural \( n \)).

```python
function pow(x, n)
    r = 1
    while n > 0
        n -= 1
        r *= x
    end
    return r
end
```

Typical AD systems use a tracing approach based on operator overloading. The input \( x \) is wrapped in a new object which overloads methods such as multiplication (\( \times \)). \( x \times y \)
no longer just multiplies \( x \) and \( y \) but records the operation and its inputs, effectively creating a graph of all basic operations in the program—equivalent to a Wengert list. Invoking \( y = \text{pow}(x, 4) \) then records the following set of basic operations.

\[
y = (((((1 \times x) \times x) \times x) \times x)
\]

The tracing technique is effectively partial evaluation; a language with rich semantics (control flow, data structures, function calls) is heavily specialised on an input to yield a program in a much simpler language (the Wengert list) that can be differentiated.

Simple or not, a program requires evaluation. Tracing AD tools are further split by whether they interpret the trace (“dynamic” frameworks) or compile it (“static” frameworks) (Neubig et al., 2017).

Dynamic approaches typically interleave tracing with evaluation of the primal, and have the benefit of preserving the host language’s expressive semantics. But they must pay the heavy cost of building and manipulating the graph anew at every iteration, and applying optimisations would cost more time than it saves (Paszke et al., 2017). These problems are increasingly important as accelerators become faster than the languages driving them, and optimisations such as operator fusion are needed to get state-of-the-art performance (Jiang et al., 2018).

Static systems evaluate the host code only once, record a graph and evaluate it instead of the original program. This comes at a high cost to expressiveness: the graph we recorded for \( \text{pow}(x, 4) \) above can only calculate \( x^4 \), and if we want richer behaviour we must have mechanisms to insert control flow into the tape. A further fundamental challenge is that traces are an extremely inefficient program representation. The size of the trace for a loop like the above is \( \text{size of loop body} \times (\text{number of iterations}) \), leading to a large amount of redundant work for an optimiser; nested loops generate exponentially large traces. Given the infeasibility of running \( O(n^2) \) compiler analysis on these graphs, these systems are still interpreted in practice (Abadi et al., 2016)—negating their main theoretical benefit.

These limitations are not fundamental to AD, but instead are limitations of the symbolic form or language that we differentiate—the Wengert list. It would be far more effective to generalise this language, so that it is directly capable of expressing richer programs which can then be fully and efficiently compiled. Happily, just such a generalisation exists via Static Single Assignment (SSA) form.

### 3 Static Single Assignment

#### 3.1 Generalising the Wengert List

SSA form (Cytron et al., 1991) generalises the Wengert list with goto-based control flow, while preserving the explicit data flow that makes analysis straightforward. The primal for the function \( f \) above looks as follows in SSA notation, with unique variables labelled \( %1, %2 \) and so on.\(^1\)

\[
\begin{align*}
%1, %2 & \leftarrow f(\cdot, y, 2) \\
%3, %4 & \leftarrow f(+, x, %1) \\
%5, %6 & \leftarrow f(/, x, %3)
\end{align*}
\]

In the adjoint, the important difference from the notation above is the use of underlined references like \( %6 \), which we refer to as alphas. They allow the adjoint code to reuse values from the primal computation without ambiguity, and will be generalised in the case of control flow.

\[
\begin{align*}
%1, %2 & \leftarrow %6(1) \\
%3, %4 & \leftarrow %4(2) \\
%5 & \leftarrow %1 + %3 \\
%6 & \leftarrow %2(4)
\end{align*}
\]

To see the effect of control flow, consider a branching function.

\[
f(x) = \begin{cases} 
  x & x > 0 \\
  0.01x & \text{otherwise}
\end{cases}
\]

In SSA form we explicitly test the condition and use a \texttt{goto} to skip the computation of \( 0.01x \) if it is not necessary. \( \phi \) functions are used to select values from previous blocks; if block 2 ran then the \( \phi \) will return the value of \( %2 \), otherwise it just returns \( x \) unmodified.\(^2\) The Wengert-list-like code between labels and \texttt{goto} instructions is referred to as a basic block.

```plaintext
block #1:
  %1 \leftarrow x > 0
  \texttt{goto} #3 \text{ if } %1

block #2:
  %2 \leftarrow 0.01x

block #3:
  %3 \leftarrow \phi(#1 \rightarrow x, #2 \rightarrow %2)

\texttt{return} %3
```

\(^1\)For notational convenience we extend SSA with multiple return values, which can be simulated with tuples.

\(^2\)Though it looks vaguely like BASIC or assembler, the lack of registers or mutable bindings makes SSA closer to a functional representation; basic blocks are equivalent to a set of mutually recursive closures (Appel, 1998).
Primal code is created much as before. To construct the adjoint, observe that unrolling the adjoint must be equivalent to constructing the adjoint for an unrolled primal. Thus, all basic blocks must be run in reverse order; there is an iteration of an adjoint block for each primal one. To achieve this we invert the primal’s control flow graph (CFG) and insert dummy \( \phi \) nodes into the primal to record and replay control flow in reverse. After this the basic blocks themselves can be differentiated.

As with the Wengert list, data flow in the adjoint is reversed; a primal SSA definition \( \%x \) corresponds to the single use of the gradient \( \%x \) with a backpropagator, and uses of \( \%x \) correspond to the creation of contributions to the gradient. As SSA definitions dominate their uses, so gradient uses post-dominate their contributions. The complication is that data flow may cross between basic blocks, and a usage of \( \%x \) may not actually execute depending on control flow. The adjoint must therefore contain appropriate \( \phi \) nodes and only take into account gradients that dynamically reach the current block. For the purpose of finding reaching gradients of \( \%x \), primal \( \phi \) nodes involving \( \%x \) can be treated as equivalent to identity(\( \%x \)).

SSA definitions may take on different values in each iteration of a primal block; alpha nodes refer to the value in the corresponding primal iteration. Given the reversed block order the right semantics can be implemented by storing values on a stack, and alpha nodes are then resolved by popping from the stack (Giering & Kaminski, 1998). The values could equally well be recomputed, and mixed approaches are able to make time-space tradeoffs (Hascoet & Pascual, 2013).

The primal thus looks as follows, adding the \( \mathcal{J} \) call and dummy \( \phi \) node at \( \%4 \).

```plaintext
block #1:
    %1 ← x > 0
    goto #3 if %1
block #2:
    %2, %3 ← \mathcal{J}(x, 0.01, x)
block #3:
    %4 ← \phi(#1 → false, #2 → true)
    %5 ← \phi(#1 → x, #2 → %2)
    return %5
```

In the adjoint code we must only apply the backpropagator \( \%3 \) to the incoming gradient \( \bar{y} \) if block 2 actually ran. We use \( \%4 \) to record what control flow happened, and then insert a \( \phi \) node to select the correct gradient of \( x \).

```plaintext
block #1:
    goto #3 if not %4
block #2:
    %1 ← %3(\bar{y})
    goto #3
block #3:
    %2 ← \phi(#1 → \bar{y}, #2 → %1)
    return %2
```

For a more complex example of these rules in practice we take the definition of \( \text{pow} \) above. The primal code illustrates how loops are represented in SSA form, via \( \phi \) nodes. Both relevant variables, \( r \) and \( n \), are explicitly carried between the two blocks comprising the loop.

```plaintext
block #1:
    %1 ← \phi(#0 → false, #2 → true)
    %2 ← \phi(#0 → 1, #2 → %6)
    %3 ← \phi(#0 → n, #2 → %5)
    %4 ← %3 > 0
    goto #3 if not %4
block #2:
    %5 ← %3 - 1
    %6, %7 ← \mathcal{J}(x, %2, x)
    goto #1
block #3:
    return %2
```

In the adjoint code, we again have two \( \phi \) functions in the loop header, effectively tracking \( \bar{x} \) (%1) and \( \bar{r} \) (%2). Block 1 has two predecessors, block 2 and the implicit block 0 (which corresponds to the return block in the primal). Only \( r \) is used in that block (as a return value), so \( \bar{x} \) has no gradient contribution and must be initialised to 0. \( x \) is used once in each iteration of the loop, so we accumulate \( \bar{x} \) across all
3.2 Handling Language Features

The SSA transform allows us to handle a large set of syntactic language constructs uniformly. However, in real-world programs the IR does not only contain numerical operations, but also many supporting functions such as for modifying state or manipulating data structures. We need not handle these features specially, but can instead treat these as additional primitives, defining appropriate backpropagators for them.

The most fundamental data structure is the cons cell, a tuple of two values like $C = (x_1, x_2)$. If we call $\text{first}(C)$ to retrieve the first element we must then find the gradient with respect to $C$ in the adjoint program. We create an adjoint object $\bar{C}$, which mirrors the structure of $C$ while storing the gradient of each internal element $(\bar{x}_1, \bar{x}_2)$. Summing adjoint objects sums the elements. The backpropagators for operations on $C$ are as follows.

| Function | Backpropagator |
|----------|----------------|
| $C = \text{cons}(x_1, x_2)$ | $\text{first}(\bar{C}), \text{second}(\bar{C})$ |
| $y = \text{first}(C)$ | $\text{cons}(\bar{y}, 0)$ |
| $y = \text{second}(C)$ | $\text{cons}(0, \bar{y})$ |

We can now differentiate any function of cons cells. Any other data structure differs only in number of fields or names of accessor functions.

To handle mutation, consider a one-element “box” structure $B$. We can get$(B)$ to retrieve the current stored value, and set$(B, x)$ to erase that value and replace it with $x$. The adjoint object $\bar{B}$ is also a box, which we retrieve via lookup rather than by backpropagator return values. The backpropagators are as follows.

\[
\begin{align*}
\text{block #1:} & \\
%1 & \leftarrow \phi(#0 \rightarrow 0, #2 \rightarrow %5) \\
%2 & \leftarrow \phi(#0 \rightarrow \bar{y}, #2 \rightarrow %3) \\
\text{goto} & \ #4 \text{ if not } %1 \\
\text{block #2:} & \\
%3, %4 & \leftarrow \%7(%2) \\
%5 & \leftarrow %1 + %4 \\
\text{goto} & \ #2 \\
\text{block #3:} & \\
\text{return} & \ %2, 0
\end{align*}
\]

A mutable cons can be seen as a boxed cons or a cons of boxes; in either case it generalises similarly to other mutable data structures. One caveat: types such as arrays may be captured by primitive backpropagators, and if the value is changed when the backpropagator runs it will be incorrect. Arrays must therefore either be immutable, be copied on capture, or have mutations recorded and reversed during the adjoint program.

In the presence of control flow, our AD implementation emits mutable stacks. Supporting mutation ensures that the AD can consume its own output, thus allowing higher-order derivatives via nested application of $\mathcal{J}$ (as in $\mathcal{J}(\mathcal{J}(f, f, x))$).

Closures are just objects with a call method; the fields of the object represent the closure’s environment. When calling closures we need to recognise a hidden zeroth argument, the closure itself, and produce an adjoint for that object. In our compiler all functions actually accept this hidden argument—which may be empty as a special case—so both closures and higher-order functions are supported with no extra effort.

4 Optimisation & Compilation

4.1 Interaction with Julia’s Compiler

It is not enough to differentiate code in principle; the approach needs to work in practice, and in particular be feasible to compile and execute efficiently. A compiler framework must be able to handle the generated code effectively and ultimately produce high-quality machine code. Our implementation in Zygote is designed to interact well with the Julia’s relatively simple compiler, and many of the principles are applicable to other languages.

In Zygote, the AD transform is entirely syntactic, and has constraints similar to a Lisp macro (albeit operating with dynamic rather than lexical extent); its compiler interception is similar to that of the Cassette tool (Revels, 2018a). Julia’s dynamic semantics mean that all function and gradient definitions are (semantically) resolved only at runtime; in general the definition of $f$ and its backpropagator in $\mathcal{J}(f, x, y)$ is unknown and could even be different each time the code is run. A concrete consequence of this is that we capture backpropagators rather than numerical values directly.

The adjoint code is nevertheless amenable to Julia’s standard optimisation heuristics, the most important of which is type inference. Consider the case where the definition of $f$ can be inferred statically, as in the $r * x$ in the
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example given above. Since the structure of the backpropagator is thus also known, we can store just the numerical contents (r and x) compactly in memory with no type tags or pointers, and inline the definition of the backpropagator at its call site. Indeed, if ∗ had instead been +, the backpropagator would be empty, and the compiler could elide the allocation of the stack entirely.

Note that the backpropagator closure for pow contains (stacks of) backpropagators for the functions it calls, and so on. This can be seen as a kind of tape whose structure defines the adjoint program. However, the stack-based design makes it crucially different from the tapes in other systems: our “tape” has the structure of the static call graph of the program, not the dynamic call graph (as in the traces described in 2.3). This crucial property is what enables Zygote’s adjoint code to be effectively statically analysed.

4.2 Results

Julia’s introspection tools can be used to check that generated output is reasonable. Firstly, we confirm that the code type infers correctly. For example we show that Julia is able to fully infer the adjoint of a simple neural network. This works just as well on larger models such as VGG19, and this level of static analysis is what enables us to target TPUs without tracing [work under preparation].

```julia
loss(m, x) = sum(m(x))
m = Chain(Dense(10,5,relu),Dense(5,2))
x = rand(10)
@code_typed(gradient(loss, m, x))
# Tuple{NamedTuple{(:layers,),Tuple{}}},Array{Float64,1}
```

This type is verbose because it is constructed, by compile-time reflection, as the adjoint of the Chain struct. Since Chain and Dense are functions that happen to have differentiable parameters, this also demonstrates the object-closure relationship described above. Note also that the gradient of f—the activation function of each layer—is statically inferred as non-differentiable; its derivative is always nothing.

After optimisation, the code for gradient(pow, 2, 3) is similar to the following (converted to high-level Julia code for ease of reading).

```julia
function grad_pow(x, n)
r = 1
Bs = Tuple{Int,Int}[]
while n > 0
    push!(Bs, (r, x))
r *= x
    n -= 1
end
dx = 0
dr = 1
for i = length(Bs):-1:1
    (r, x) = Bs[i]
dx += dr*r
dr = dr*x
end
return dx
end
```

Stacks have low overhead at less than 10 nanoseconds per operation on a typical CPU; this is noticeable compared to scalar numerical operations, but generally negligible in array code. It compares especially favourably to constructing and differentiating a program trace, as in other dynamic AD systems, which has typical overhead in the microseconds per operation (PyTorch Team, 2018).

To confirm this in more realistic cases, Table 2 provides a set of simple benchmarks between a plain Julia forward pass, Zygote, PyTorch (Paszke et al., 2017) and ReverseDiff (Revels, 2018b) (a tracing-based AD with optional compilation). These mix scalar (sincos and loop) and vector examples to both stress-test AD overhead and show more realistic speedups, respectively.

The case without control flow does not even require a stack, and Zygote can match optimised, hand-written gradients in many cases. In cases such as f(x) = 5x+3, Julia will type infer the entire call chain, resolve the backpropagators for ∗ and +, and inline through all the abstraction (166 different function calls in total) to produce code with only a few integer operations. LLVM then runs constant propagation and produces the following code:

```julia
define i64 @"julia_#625_38792"(i64) {
  top:
    ret i64 5
}
```

While LLVM is able to perform powerful optimisations, its knowledge is limited to scalar functions. But there are an increasing number of tensor-aware IRs and compiler stacks (XLA, 2018; Cyphers et al., 2018; Wei et al., 2017), and Zygote’s approach to AD makes it much easier to either target these for more advanced optimisations or to apply
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Table 2. Benchmarks on some simple functions.

| BENCHMARK                  | FORWARD | ZYGOTE  | PYTORCH | REVERSEDIFF |
|----------------------------|---------|---------|---------|-------------|
| SinCos                     | 15.94NS | 20.74NS | 69.9µs  | 670.2NS     |
| Loop                      | 4.17µs  | 29.5µs  | 17.5µs  | 170.9µs     |
| LogSumExp                 | 0.96µs  | 2.74µs  | 219.1µs | 15.9µs      |
| Logistic Regression       | 4.67µs  | 17.6µs  | 142.2µs | 89.9µs      |
| 2-LAYER MNIST MLP         | 27.7µs  | 207.0µs | 368.6µs | N/A         |

them on Julia’s IR directly—without sacrificing flexibility and abstraction for the researcher.

5 CONCLUSION

This paper presents a system for differentiation via the $\mathcal{J}$ function and backpropagators, and uses these to build a system for differentiation via the $\mathcal{J}$ function and backpropagators. Current AD systems which use program-tracing approaches face a fundamental tradeoff between performance and flexibility, but we hope to have shown that this tradeoff is not fundamental. Our new AD, Zygote, supports a full range of language features—from control flow to macros—while producing highly optimised code.

By transforming SSA-form IR we can differentiate rich and expressive programs with extremely low run-time overhead, while opening up opportunities for even more optimisation in future. As SSA is used as an intermediate representation (IR) by many recent language compilers, differentiation could be added as a first-class language feature to many modern compiled languages, enabling truly differentiable programming.

Given the increasing complexity and performance requirements of machine learning models, research will increasingly be enabled or limited by the capabilities of language and compiler technology, including AD. We hope the community will continue pushing the frontiers of that compiler technology forward, and machine learning with it.

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