Automatic Differentiation in Machine Learning: a Survey

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Abstract

Derivatives, mostly in the form of gradients and Hessians, are ubiquitous in machine learning. Automatic differentiation (AD), also called algorithmic differentiation or simply "autodiff", is a family of techniques similar to but more general than backpropagation for efficiently and accurately evaluating derivatives of numeric functions expressed as computer programs. AD is a small but established field with applications in areas including computational fluid dynamics, atmospheric sciences, and engineering design optimization. Until very recently, the fields of machine learning and AD have largely been unaware of each other and, in some cases, have independently discovered each other's results. Despite its relevance, general-purpose AD has been missing from the toolbox of the machine learning community, a situation slowly changing with its ongoing adoption in mainstream machine learning frameworks. We survey the intersection of AD and machine learning, cover applications where AD has direct relevance, and address the main techniques of implementation. By precisely defining the main differentiation techniques and their interrelationships, we aim to bring clarity to the usage of terms "autodiff", "automatic differentiation", and "symbolic differentiation" as these are encountered more and more in machine learning settings.

Keywords: Backpropagation, Gradient-Based Optimization

1. Introduction

Methods for the computation of derivatives in computer programs can be classified into four categories: (1) manually working out derivatives and coding them; (2) numerical differentiation using finite difference approximations; (3) symbolic differentiation using expression manipulation in computer algebra systems such as Mathematica, Maxima, and Maple; and (4) automatic differentiation, also called algorithmic differentiation, which is the subject matter of this paper.

Conventionally, many methods in machine learning have required the evaluation of derivatives and most of the traditional learning algorithms have relied on the computation of gradients and Hessians of an objective function (Sra et al., 2011). When introducing new models, machine learning researchers have spent considerable effort on the manual derivation of analytical derivatives to subsequently plug these into standard optimization procedures such as L-BFGS (Zhu et al., 1997) or stochastic gradient descent (Bottou, 1998). Manual differentiation is time consuming and prone to error. Of the other alternatives, numerical differentiation is simple to implement, but scales poorly for gradients and can be highly inaccurate due to round-off and truncation errors (Jerrell, 1997). Symbolic differentiation addresses the weaknesses of both the manual and numerical methods, but often results in complex and cryptic expressions plagued with the problem of "expression swell" (Corliss, 1988). Furthermore, manual and symbolic methods require models to be expressed as closed-form mathematical formulae, ruling out algorithmic control flow and/or severely limiting expressivity.

We are concerned with the powerful fourth technique, automatic differentiation (AD), which works by systematically applying the chain rule of differential calculus at the elementary operator level. Despite its widespread use in other fields, general-purpose AD has been underused by the machine learning community until very recently. Following the emergence of deep learning (LeCun et al., 2015; Goodfellow et al., 2016) as the state-of-the-art in many machine learning tasks and the modern workflow based on rapid prototyping and code reuse in frameworks such as Theano (Bastien et al., 2012), Torch (Collobert et al., 2011), and TensorFlow (Abadi et al., 2016), the situation is slowly changing where projects such as autograd, torch-autograd, and PyTorch are leading the way in bringing general-purpose AD to the mainstream.

The term "automatic" in AD is somewhat a misnomer that can cause confusion among machine learning practitioners to put the label "automatic differentiation", or just "autodiff" on any method or tool that does not involve manual differentiation, without giving due attention to the underlying mechanism. We would like to stress that AD as a term refers to a specific family of techniques that compute derivatives through accumulation of values during code execution and generate numerical derivative evaluations rather than derivative expressions. This allows accurate evaluation of derivatives at machine precision with only a small constant factor of overhead and ideal asymptotic efficiency. In contrast with the effort involved in arranging code as closed-form expressions under the syntactic and semantic constraints of symbolic differentiation, AD can be applied to regular code with minimal change,

^{1.} See, e.g., https://justindomke.wordpress.com/2009/02/17/automatic-differentiation-the-most-criminally-underused

^{2.} https://github.com/HIPS/autograd

^{3.} https://github.com/twitter/torch-autograd

^{4.} http://pytorch.org/

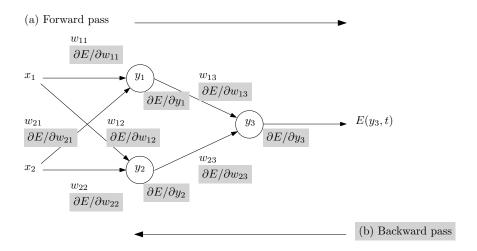


Figure 1: Overview of backpropagation. (a) Training inputs x_i are fed forward, generating corresponding activations y_i . Error between the actual output y_3 and the target output t is computed. (b) The error is propagated backward, giving the gradient $\nabla_{w_{ij}} E$, which is subsequently used in a gradient descent procedure. The gradient with respect to inputs $\nabla_{x_i} E$ can be also computed in the same backward pass.

allowing branching, loops, and recursion. Because of this generality, AD has been applied to computer simulations in industry and academia and found applications in fields including engineering design optimization (Forth and Evans, 2002; Casanova et al., 2002), computational fluid dynamics (Müller and Cusdin, 2005; Thomas et al., 2006; Bischof et al., 2006), physical modeling (Ekström et al., 2010), optimal control (Walther, 2007), structural mechanics (Haase et al., 2002), atmospheric sciences (Carmichael and Sandu, 1997; Charpentier and Ghemires, 2000), and computational finance (Bischof et al., 2002; Capriotti, 2011).

AD and machine learning practice are conceptually very closely related: consider the backpropagation algorithm for training neural networks, which has a colorful history of having been reinvented at various times by independent researchers (Griewank, 2012). It has been one of the most studied and used training algorithms since the day it became popular mainly through the work of Rumelhart et al. (1986). In simplest terms, backpropagation models learning as gradient descent in neural network weight space, looking for the minimum of an objective function. This is accomplished by the backward propagation of the objective value at the output (Figure 1) utilizing the chain rule to compute the gradient of the objective with respect to each weight. The resulting algorithm is essentially equivalent to transforming the network evaluation function composed with the objective function under reverse mode automatic differentiation, which, as we shall see, actually generalizes the backpropagation idea. Thus, a modest understanding of the mathematics underlying backpropagation already provides one with the sufficient background for grasping AD techniques.

In this paper we review AD from a machine learning perspective, covering its origins, applications in machine learning, and methods of implementation. Along the way, we also aim to dispel some misconceptions that we believe have impeded wider recognition of AD by the machine learning community. In Section 2 we start by explicating how AD differs from numerical and symbolic differentiation. Section 3 gives an introduction to the AD technique and its forward and reverse accumulation modes. Section 4 discusses the role of derivatives in machine learning and examines cases where AD has relevance. Section 5 covers various implementation approaches and general-purpose AD tools, followed by Section 6 where we discuss future directions.

2. What AD Is Not

Without proper introduction, one might assume that AD is either a type of numerical or symbolic differentiation. Confusion can arise because AD does in fact provide only numerical values of derivatives (as opposed to derivative expressions) and it does so by using symbolic rules of differentiation (but keeping track of derivative values as opposed to the resulting expressions), giving it a two-sided nature that is partly symbolic and partly numerical (Griewank, 2003). We start by emphasizing how AD is different from, and in several aspects superior to, these two commonly encountered techniques of computing derivatives.

2.1 AD Is Not Numerical Differentiation

Numerical differentiation is the finite difference approximation of derivatives using values of the original function evaluated at some sample points (Burden and Faires, 2001) (Figure 2). In its simplest form, it is based on the limit definition of a derivative. For example, for a multivariate function $f: \mathbb{R}^n \to \mathbb{R}$, one can approximate the gradient $\nabla f = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}\right)$ using

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \frac{f(\mathbf{x} + h\mathbf{e}_i) - f(\mathbf{x})}{h} , \qquad (1)$$

where \mathbf{e}_i is the *i*-th unit vector and h > 0 is a small step size. This has the advantage of being uncomplicated to implement, but the disadvantages of performing O(n) evaluations of f for a gradient in n dimensions and requiring careful consideration in selecting the step size h.

Numerical approximations of derivatives are inherently ill-conditioned and unstable,⁵ with the exception of complex variable methods that are applicable to a limited set of holomorphic functions (Fornberg, 1981). This is due to the introduction of truncation⁶ and round-off⁷ errors inflicted by the limited precision of computations and the chosen value

^{5.} Using the limit definition of the derivative for finite difference approximation commits both cardinal sins of numerical analysis: "thou shalt not add small numbers to big numbers", and "thou shalt not subtract numbers which are approximately equal".

^{6.} Truncation error is the error of approximation, or inaccuracy, one gets from h not actually being zero. It is proportional to a power of h.

^{7.} Round-off error is the inaccuracy one gets from valuable low-order bits of the final answer having to compete for machine-word space with high-order bits of $f(\mathbf{x}+h\mathbf{e}_i)$ and $f(\mathbf{x})$ (Eq. 1), which the computer has to store just until they cancel in the subtraction at the end. Round-off error is inversely proportional to a power of h.

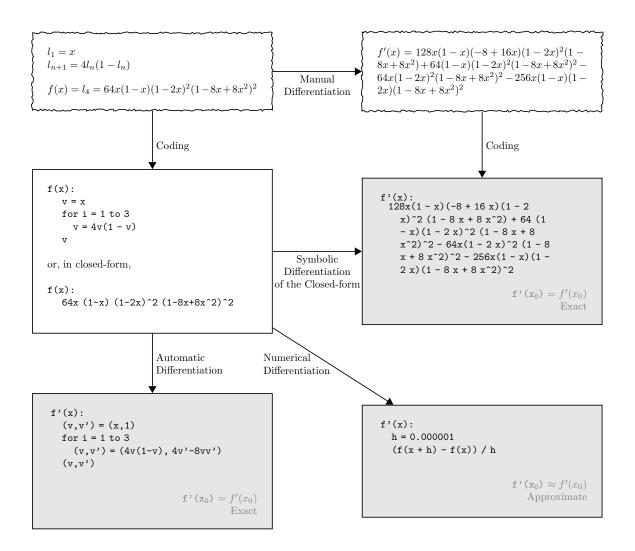


Figure 2: The range of approaches for differentiating mathematical expressions and computer code, looking at the example of a truncated logistic map (upper left). Symbolic differentiation (center right) gives exact results but requires closed-form input and suffers from expression swell; numerical differentiation (lower right) has problems of accuracy due to round-off and truncation errors; automatic differentiation (lower left) is as accurate as symbolic differentiation with only a constant factor of overhead and support for control flow.

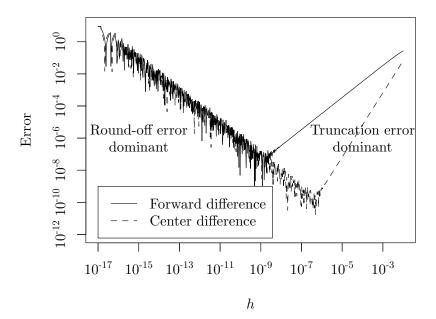


Figure 3: Error in the forward (Eq. 1) and center difference (Eq. 2) approximations as a function of step size h, for the derivative of the truncated logistic map $f(x) = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$. Plotted errors computed using $E_{\text{forward}}(h,x_0) = \left|\frac{f(x_0+h)-f(x_0)}{h} - \frac{d}{dx}f(x)\right|_{x_0}\right|$ and $E_{\text{center}}(h,x_0) = \left|\frac{f(x_0+h)-f(x_0-h)}{2h} - \frac{d}{dx}f(x)\right|_{x_0}$ at $x_0 = 0.2$.

of the step size h. Truncation error tends to zero as $h \to 0$. However, as h is decreased, round-off error increases and becomes dominant (Figure 3).

Techniques have been developed to mitigate the approximation errors in numerical differentiation, such as using a center difference approximation

$$\frac{\partial f(\mathbf{x})}{\partial x_i} = \frac{f(\mathbf{x} + h\mathbf{e}_i) - f(\mathbf{x} - h\mathbf{e}_i)}{2h} + O(h^2) , \qquad (2)$$

where the first-order errors cancel and one effectively moves the truncation error from first-order to second-order in h.⁸ For the one-dimensional case, it is just as costly to compute the forward difference (Eq. 1) and the center difference (Eq. 2), requiring only two evaluations of f. However, with increasing dimensionality, a trade-off between accuracy and performance is faced, where computing a Jacobian matrix of a function $f: \mathbb{R}^n \to \mathbb{R}^m$ requires 2mn evaluations.

Other techniques for improving numerical differentiation, including higher-order finite differences, Richardson extrapolation to the limit (Brezinski and Zaglia, 1991), and differential quadrature methods using weighted sums (Bert and Malik, 1996), have increased

^{8.} This does not avoid either of the cardinal sins, and is still highly inaccurate due to truncation.

computational complexity, do not completely eliminate approximation errors, and remain highly susceptible to floating point truncation.

2.2 AD Is Not Symbolic Differentiation

Symbolic differentiation is the automatic manipulation of expressions for obtaining derivative expressions (Grabmeier and Kaltofen, 2003) (Figure 2), carried out by applying transformations representing rules of differentiation such as

$$\frac{d}{dx}(f(x) + g(x)) \rightsquigarrow \frac{d}{dx}f(x) + \frac{d}{dx}g(x)$$

$$\frac{d}{dx}(f(x)g(x)) \rightsquigarrow \left(\frac{d}{dx}f(x)\right)g(x) + f(x)\left(\frac{d}{dx}g(x)\right) .$$
(3)

When formulae are represented as data structures, symbolically differentiating an expression tree is a perfectly mechanistic process, already considered subject to mechanical automation at the very inception of calculus (Leibniz, 1685). This is realized in modern computer algebra systems such as Mathematica, Maxima, and Maple and machine learning frameworks such as Theano.

In optimization, symbolic derivatives can give valuable insight into the structure of the problem domain and, in some cases, produce analytical solutions of extrema (e.g., solving for $\frac{d}{dx}f(x)=0$) that can eliminate the need for derivative calculation altogether. On the other hand, symbolic derivatives do not lend themselves to efficient runtime calculation of derivative values, as they can get exponentially larger than the expression whose derivative they represent.

Consider a function h(x) = f(x)g(x) and the multiplication rule in Eq. 3. Since h is a product, h(x) and $\frac{d}{dx}h(x)$ have some common components, namely f(x) and g(x). Note also that on the right hand side, f(x) and $\frac{d}{dx}f(x)$ appear separately. If we just proceeded to symbolically differentiate f(x) and plugged its derivative into the appropriate place, we would have nested duplications of any computation that appears in common between f(x) and $\frac{d}{dx}f(x)$. Hence, careless symbolic differentiation can easily produce exponentially large symbolic expressions which take correspondingly long to evaluate. This problem is known as expression swell (Table 1).

When we are concerned with the accurate numerical evaluation of derivatives and not so much with their actual symbolic form, it is in principle possible to significantly simplify computations by storing only values of intermediate subexpressions in memory. Moreover, for further efficiency, we can interleave as much as possible the differentiation and simplification steps. This interleaving idea forms the basis of AD and provides an account of its simplest form: apply symbolic differentiation at the elementary operation level and keep intermediate numerical results, in lockstep with the evaluation of the main function. This is AD in the forward accumulation mode, which we shall introduce in the following section.

3. AD and Its Main Modes

In its most basic description, AD relies on the fact that all numerical computations are ultimately compositions of a finite set of elementary operations for which derivatives are

Table 1: Iterations of the logistic map $l_{n+1} = 4l_n(1 - l_n)$, $l_1 = x$ and the corresponding derivatives of l_n with respect to x, illustrating expression swell.

n	l_n	$\frac{d}{dx}l_n$	$\frac{d}{dx}l_n$ (Simplified form)
1	x	1	1
2	4x(1-x)	4(1-x)-4x	4-8x
3	$16x(1-x)(1-2x)^2$	$ 16(1-x)(1-2x)^2 - 16x(1-2x)^2 - 64x(1-x)(1-2x) $	$16(1 - 10x + 24x^2 - 16x^3)$
4	$64x(1-x)(1-2x)^2$ $(1-8x+8x^2)^2$	$ 128x(1-x)(-8+16x)(1-2x)^2(1-8x+8x^2)+64(1-x)(1-2x)^2(1-8x+8x^2)^2-64x(1-2x)^2(1-8x+8x^2)^2-256x(1-x)(1-2x)(1-8x+8x^2)^2 $	$64(1 - 42x + 504x^2 - 2640x^3 + 7040x^4 - 9984x^5 + 7168x^6 - 2048x^7)$

known (Verma, 2000; Griewank and Walther, 2008). Combining the derivatives of the constituent operations through the chain rule gives the derivative of the overall composition. Usually these elementary operations include the binary arithmetic operations, the unary sign switch, and transcendental functions such as the exponential, the logarithm, and the trigonometric functions.

On the left hand side of Table 2 we see the representation of the computation $y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$ as an evaluation trace of elementary operations—also called a Wengert list (Wengert, 1964). We adopt the three-part notation used by Griewank and Walther (2008), where a function $f : \mathbb{R}^n \to \mathbb{R}^m$ is constructed using intermediate variables v_i such that

- variables $v_{i-n} = x_i$, i = 1, ..., n are the input variables,
- variables v_i $i=1,\ldots,l$ are the working (intermediate) variables, and
- variables $y_{m-i} = v_{l-i}, i = m-1, \ldots, 0$ are the output variables.

Figure 4 shows the given trace of elementary operations represented as a computational graph (Bauer, 1974), useful in visualizing dependency relations between intermediate variables.

Evaluation traces form the basis of the AD techniques. An important point to note here is that AD can differentiate not only mathematical expressions in the classical sense, but also algorithms making use of control flow such as branching, loops, recursion, and procedure calls, giving it an important advantage over symbolic differentiation which severely limits such expressivity. This is thanks to the fact that any numeric code will eventually result in a numeric execution trace with particular values of the input, intermediate, and output variables, which are the only things one needs to know for computing derivatives using chain rule composition, regardless the specific control flow path that was taken during execution. Another way of expressing this is that AD is blind with respect to any operation, including control flow statements, which do not directly alter numeric values.

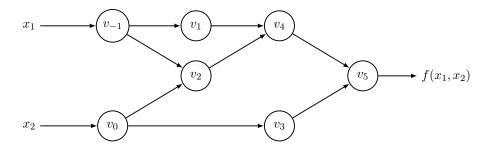


Figure 4: Computational graph of the example $f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$. See the primal trace in Tables 2 or 3 for the definitions of the intermediate variables $v_{-1} \dots v_5$.

3.1 Forward Mode

AD in forward accumulation mode⁹ is the conceptually most simple type. Consider the evaluation trace of the function $f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$ given on the left-hand side in Table 2 and in graph form in Figure 4. For computing the derivative of f with respect to x_1 , we start by associating with each intermediate variable v_i a derivative

$$\dot{v}_i = \frac{\partial v_i}{\partial x_1} \ .$$

Applying the chain rule to each elementary operation in the forward primal trace, we generate the corresponding tangent (derivative) trace, given on the right-hand side in Table 2. Evaluating the primals v_i in lockstep with their corresponding tangents \dot{v}_i gives us the required derivative in the final variable $\dot{v}_5 = \frac{\partial y}{\partial x_1}$.

This generalizes naturally to computing the Jacobian of a function $f: \mathbb{R}^n \to \mathbb{R}^m$ with n independent (input) variables x_i and m dependent (output) variables y_j . In this case, each forward pass of AD is initialized by setting only one of the variables $\dot{x}_i = 1$ (in other words, setting $\dot{\mathbf{x}} = \mathbf{e}_i$, where \mathbf{e}_i is the i-th unit vector). A run of the code with specific input values $\mathbf{x} = \mathbf{a}$ would then compute

$$\dot{y}_j = \frac{\partial y_j}{\partial x_i} \Big|_{\mathbf{x} = \mathbf{a}}, \ j = 1, \dots, m ,$$

giving us one column of the Jacobian matrix

$$\mathbf{J}_{f} = \begin{bmatrix} \frac{\partial y_{1}}{\partial x_{1}} & \cdots & \frac{\partial y_{1}}{\partial x_{n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_{m}}{\partial x_{1}} & \cdots & \frac{\partial y_{m}}{\partial x_{n}} \end{bmatrix} \Big|_{\mathbf{x} = \mathbf{a}}$$

evaluated at point a. Thus, the full Jacobian can be computed in n evaluations.

^{9.} Also called tangent linear mode.

Table 2: Forward mode AD example, with $y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$ evaluated at $(x_1, x_2) = (2, 5)$ and setting $\dot{x}_1 = 1$ to compute $\frac{\partial y}{\partial x_1}$. The original forward evaluation of the primals on the left is augmented by the tangent operations on the right, where each line supplements the original directly to its left.

Forward Primal Trace			Forward Tangent (Derivative) Trace				
$v_{-1} = x_1$	=2		\dot{v}_{-}	$\dot{x}_1 = \dot{x}_1$	= 1		
$v_0 = x_2$	= 5	ı	\dot{v}_0	$=\dot{x}_2$	=0		
$v_1 = \ln v_{-1}$	$= \ln 2$		\dot{v}_1	$=\dot{v}_{-1}/v_{-1}$	= 1/2		
$v_2 = v_{-1} \times v_0$	$=2\times5$		\dot{v}_2	$=\dot{v}_{-1}\times v_0+\dot{v}_0\times v_{-1}$	$= 1 \times 5 + 0 \times 2$		
$v_3 = \sin v_0$	$=\sin 5$		\dot{v}_3	$=\dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$		
$v_4 = v_1 + v_2$	= 0.693 + 10		\dot{v}_4	$=\dot{v}_1+\dot{v}_2$	=0.5+5		
	= 10.693 + 0.959	\downarrow	\dot{v}_5	$=\dot{v}_4-\dot{v}_3$	=5.5-0		
$y = v_5$	= 11.652		$\dot{m{y}}$	$=\dot{v}_{5}$	= 5.5		

Furthermore, forward mode AD provides a very efficient and matrix-free way of computing Jacobian-vector products

$$\mathbf{J}_{f} \mathbf{r} = \begin{bmatrix} \frac{\partial y_{1}}{\partial x_{1}} & \cdots & \frac{\partial y_{1}}{\partial x_{n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_{m}}{\partial x_{1}} & \cdots & \frac{\partial y_{m}}{\partial x_{n}} \end{bmatrix} \begin{bmatrix} r_{1} \\ \vdots \\ r_{n} \end{bmatrix} , \qquad (4)$$

simply by initializing with $\dot{\mathbf{x}} = \mathbf{r}$. Thus, we can compute the Jacobian-vector product in just one forward pass. As a special case, when $f: \mathbb{R}^n \to \mathbb{R}$, we can obtain the directional derivative along a given vector \mathbf{r} as a linear combination of the partial derivatives

$$\nabla f \cdot \mathbf{r}$$

by starting the AD computation with the values $\dot{\mathbf{x}} = \mathbf{r}$.

Forward mode AD is efficient and straightforward for functions $f: \mathbb{R} \to \mathbb{R}^m$, as all the derivatives $\frac{\partial y_i}{\partial x}$ can be computed with just one forward pass. Conversely, in the other extreme of $f: \mathbb{R}^n \to \mathbb{R}$, forward mode AD would require n evaluations to compute the gradient

$$\nabla f = \left(\frac{\partial y}{\partial x_1}, \dots, \frac{\partial y}{\partial x_n}\right) .$$

In general, for cases $f: \mathbb{R}^n \to \mathbb{R}^m$ where $n \gg m$, a different technique is often preferred. We will describe AD in reverse accumulation mode in Section 3.2.

3.1.1 Dual Numbers

Mathematically, forward mode AD (represented by the left- and right-hand sides in Table 2) can be viewed as using dual numbers, ¹⁰ which can be defined as formal truncated Taylor

^{10.} First introduced by Clifford (1873), with important uses in linear algebra and physics.

series of the form

$$v + \dot{v}\epsilon$$
.

Defining arithmetic on dual numbers by $\epsilon^2 = 0$ and by interpreting any non-dual number v as $v + 0\epsilon$, we see for example that

$$(v + \dot{v}\epsilon) + (u + \dot{u}\epsilon) = (v + u) + (\dot{v} + \dot{u})\epsilon,$$

$$(v + \dot{v}\epsilon)(u + \dot{u}\epsilon) = (vu) + (v\dot{u} + \dot{v}u)\epsilon,$$

in which the coefficients of ϵ conveniently mirror symbolic differentiation rules (e.g., Eq. 3). We can utilize this by setting up a regime where

$$f(v + \dot{v}\epsilon) = f(v) + f'(v)\dot{v}\epsilon \tag{5}$$

and using dual numbers as data structures for carrying the tangent value together with the primal.¹¹ The chain rule works as expected on this representation: two applications of Eq. 5 give

$$f(g(v + \dot{v}\epsilon)) = f(g(v) + g'(v)\dot{v}\epsilon)$$

= $f(g(v)) + f'(g(v))g'(v)\dot{v}\epsilon$.

The coefficient of ϵ on the right-hand side is exactly the derivative of the composition of f and g. This means that since we implement elementary operations to respect the invariant Eq. 5, all compositions of them will also do so. This, in turn, means that we can extract the derivative of a function of interest by evaluating it in this nonstandard way on an initial input with a coefficient 1 for ϵ :

$$\frac{df(x)}{dx}\Big|_{x=v}$$
 = epsilon-coefficient(dual-version $(f)(v+1\epsilon)$).

This also extends to arbitrary program constructs, since dual numbers, as data types, can be contained in any data structure. As long as no arithmetic is done on the dual number, it will just remain a dual number; and if it is taken out of the data structure and operated on again, then the differentiation will continue.

In practice, a function f coded in a programming language of choice would be fed into an AD tool, which would then augment it with corresponding extra code to handle the dual operations, so that the function and its derivative are simultaneously computed. This can be implemented through calls to a specific library, in the form of source transformation where a given source code will be automatically modified, or through operator overloading, making the process transparent to the user. We discuss these implementation techniques in Section 5.

^{11.} Just as the complex number written x + yi is represented in the computer as a pair in memory $\langle x, y \rangle$ whose two slots are reals, the dual number written $x + \dot{x}\epsilon$ is represented as the pair $\langle x, \dot{x} \rangle$.

3.2 Reverse Mode

AD in the reverse accumulation mode^{12} corresponds to a generalized backpropagation algorithm, in that it propagates derivatives backward from a given output. This is done by supplementing each intermediate variable v_i with an adjoint

$$\bar{v}_i = \frac{\partial y_j}{\partial v_i} \;,$$

which represents the sensitivity of a considered output y_j with respect to changes in v_i . In the case of backpropagation, y would be a scalar corresponding to the error E.

Derivatives are computed in the second stage of a two-stage process. In the first stage, the original function code is run *forward*, populating intermediate variables v_i and recording the dependencies in the computational graph through a bookkeeping procedure. In the second stage, derivatives are calculated by propagating adjoints \bar{v}_i in *reverse*, from the outputs to the inputs.

Returning to the example $y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$, in Table 3 we see the adjoint statements on the right-hand side, corresponding to each original elementary operation on the left-hand side. In simple terms, we are interested in computing the contribution $\bar{v}_i = \frac{\partial y}{\partial v_i}$ of the change in each variable v_i to the change in the output y. Taking the variable v_0 as an example, we see in Figure 4 that the only way it can affect y is through affecting v_2 and v_3 , so its contribution to the change in y is given by

$$\frac{\partial y}{\partial v_0} = \frac{\partial y}{\partial v_2} \frac{\partial v_2}{\partial v_0} + \frac{\partial y}{\partial v_3} \frac{\partial v_3}{\partial v_0} \qquad \text{or} \qquad \bar{v}_0 = \bar{v}_2 \frac{\partial v_2}{\partial v_0} + \bar{v}_3 \frac{\partial v_3}{\partial v_0} .$$

In Table 3, this contribution is computed in two incremental steps

$$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0}$$
 and $\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$,

lined up with the lines in the forward trace from which these expressions originate.

After the forward pass on the left-hand side, we run the reverse pass of the adjoints on the right-hand side, starting with $\bar{v}_5 = \bar{y} = \frac{\partial y}{\partial y} = 1$. In the end we get the derivatives $\frac{\partial y}{\partial x_1} = \bar{x}_1$ and $\frac{\partial y}{\partial x_2} = \bar{x}_2$ in just one reverse pass.

Compared with the straightforward simplicity of forward accumulation mode, reverse

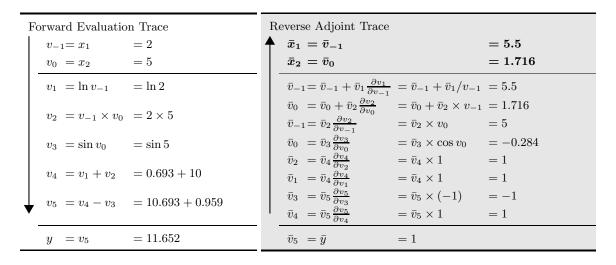
Compared with the straightforward simplicity of forward accumulation mode, reverse mode AD can, at first, appear somewhat "mysterious" (Dennis and Schnabel, 1996). Griewank and Walther (2008) argue that this is in part because of the common acquaintance with the chain rule as a mechanistic procedure propagating derivatives forward.

An important advantage of the reverse mode is that it is significantly less costly to evaluate (in terms of operation count) than the forward mode for functions with a large number of inputs. In the extreme case of $f: \mathbb{R}^n \to \mathbb{R}$, only one application of the reverse mode is sufficient to compute the full gradient $\nabla f = \left(\frac{\partial y}{\partial x_1}, \dots, \frac{\partial y}{\partial x_n}\right)$, compared with the n passes of the forward mode needed for populating the same.

In general, for a function $f: \mathbb{R}^n \to \mathbb{R}^m$, if we denote the operation count to evaluate the original function by ops(f), the time it takes to calculate the $m \times n$ Jacobian by the

^{12.} Also called adjoint or cotangent linear mode.

Table 3: Reverse mode AD example, with $y = f(x_1, x_2) = \ln(x_1) + x_1x_2 - \sin(x_2)$ evaluated at $(x_1, x_2) = (2, 5)$. After the forward evaluation of the primals on the left, the adjoint operations on the right are evaluated in reverse (cf. Figure 1). Note that both $\frac{\partial y}{\partial x_1}$ and $\frac{\partial y}{\partial x_2}$ are computed in the same reverse pass, starting from the adjoint $\bar{v}_5 = \bar{y} = \frac{\partial y}{\partial y} = 1$.



forward mode is n c ops(f), whereas the same computation can be done via reverse mode in m c ops(f), where c is a constant guaranteed to be c < 6 and typically c ~ [2,3] (Griewank and Walther, 2008). That is to say, reverse mode AD performs better when $m \ll n$.

Similar to the matrix-free computation of Jacobian-vector products with forward mode (Eq. 4), reverse mode can be used for computing the transposed Jacobian-vector product

$$\mathbf{J}_{f}^{\mathsf{T}}\mathbf{r} = \begin{bmatrix} \frac{\partial y_{1}}{\partial x_{1}} & \cdots & \frac{\partial y_{m}}{\partial x_{1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_{1}}{\partial x_{n}} & \cdots & \frac{\partial y_{m}}{\partial x_{n}} \end{bmatrix} \begin{bmatrix} r_{1} \\ \vdots \\ r_{m} \end{bmatrix} ,$$

by initializing the reverse stage with $\bar{\mathbf{y}} = \mathbf{r}$.

The advantages of reverse mode AD, however, come with the cost of increased storage requirements growing (in the worst case) in proportion to the number of operations in the evaluated function. It is an active area of research to improve storage requirements in implementations by using advanced methods such as checkpointing strategies and data-flow analysis (Dauvergne and Hascoët, 2006).

3.3 Origins of AD and Backpropagation

Ideas underlying AD date back to the 1950s (Nolan, 1953; Beda et al., 1959). Forward mode AD as a general method for evaluating partial derivatives was essentially discovered by Wengert (1964). It was followed by a period of relatively low activity, until interest in the field was revived in the 1980s mostly through the work of Griewank (1989), also

supported by improvements in modern programming languages and the feasibility of an efficient reverse mode ${\rm AD}.^{13}$

Reverse mode AD and backpropagation have an intertwined history. The essence of the reverse mode, cast in a continuous-time formalism, is the Pontryagin maximum principle (Rozonoer, 1959; Boltyanskii et al., 1960). This method was understood in the control theory community (Bryson and Denham, 1962; Bryson and Ho, 1969) and cast in more formal terms with discrete-time variables topologically sorted in terms of dependency by Werbos (1974). Speelpenning (1980) discovered reverse mode AD and gave the first implementation that was actually automatic, in the sense of accepting a specification of a computational process written in a general-purpose programming language and automatically performing the reverse mode transformation.

Incidentally, Hecht-Nielsen (1989) cites the work of Bryson and Ho (1969) and Werbos (1974) as the two earliest known instances of backpropagation. Within the machine learning community, the method has been reinvented several times, such as by Parker (1985), until it was eventually brought to fame by Rumelhart et al. (1986) and the Parallel Distributed Processing (PDP) group. The PDP group became aware of Parker's work only after their own discovery; similarly, Werbos' work was not appreciated until it was found by Parker. This tells us an interesting story of two highly interconnected research communities that have somehow also managed to stay detached during this foundational period.

4. AD and Machine Learning

In the following, we examine the main uses of derivatives in machine learning and report a selection of works where general-purpose AD has been successfully applied in a machine learning context. Areas where AD has seen use include optimization, neural networks, computer vision, natural language processing, and probabilistic inference.

4.1 Gradient-Based Optimization

Given an objective function $f: \mathbb{R}^n \to \mathbb{R}$, classical gradient descent has the goal of finding (local) minima $\mathbf{w}^* = \arg\min_{\mathbf{w}} f(\mathbf{w})$ via updates $\Delta \mathbf{w} = -\eta \nabla f$, where $\eta > 0$ is a step size. Gradient methods make use of the fact that f decreases steepest if one goes in the direction of the negative gradient. Naïve gradient descent comes with asymptotic rate of convergence, where the method increasingly "zigzags" towards the minimum in a slowing down fashion. The convergence rate is usually improved by adaptive step size techniques that adjust the step size η on every iteration (Duchi et al., 2011; Schaul et al., 2013; Kingma and Ba, 2015).

As we have seen, for large n, reverse mode AD—or backpropagation—provides a highly efficient method for computing gradients. Figure 5 and Table 4 demonstrate how gradient computation scales differently for forward and reverse mode AD and numerical differentiation, looking at the Helmholtz free energy function that has been used in AD literature for benchmarking gradient calculations (Griewank, 1989; Griewank and Walther, 2008).

^{13.} For a thorough review of the development of AD, we advise readers to refer to Rall (2006) Also see Griewank (2012) for an investigation of the origins of the reverse mode.

^{14.} See http://gbaydin.github.io/DiffSharp/examples-gradientdescent.html for an example of a general-purpose AD-based gradient descent routine using the DiffSharp library.

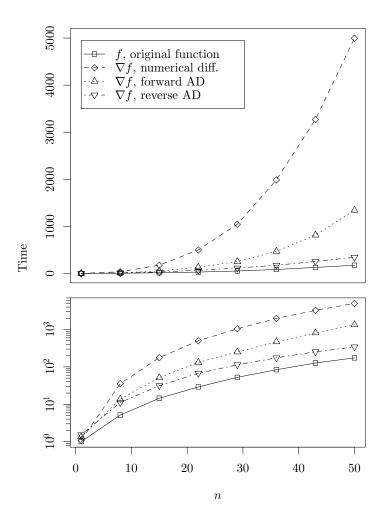


Figure 5: Evaluation time of the Helmholtz free energy function of a mixed fluid, based on the Peng-Robinson equation of state (Peng and Robinson, 1976), $f(\mathbf{x}) = RT \sum_{i=0}^{n} \log \frac{x_i}{1-\mathbf{b^T x}} - \frac{\mathbf{x^T A x}}{\sqrt{8}\mathbf{b^T x}} \log \frac{1+(1+\sqrt{2})\mathbf{b^T x}}{1+(1-\sqrt{2})\mathbf{b^T x}}, \text{ where } R \text{ is the universal gas constant, } T \text{ is the absolute temperature, } \mathbf{b} \in \mathbb{R}^n \text{ is a vector of constants, } \mathbf{A} \in \mathbb{R}^{n \times n} \text{ is a symmetric matrix of constants, and } \mathbf{x} \in \mathbb{R}^n \text{ is the vector of independent variables describing the system. The plots show the evaluation time of <math>f$ and the gradient ∇f with numerical differentiation (central difference), forward mode AD, and reverse mode AD, as a function of the number of variables n. Reported times are relative to the evaluation time of f with n = 1. The lower plot uses logarithmic scale for illustrating the behavior when n < 20. Numerical results are given in Table 4. (Code: http://gbaydin.github.io/DiffSharp/misc/Benchmarks-h-grad-v0.5.7.fsx)

Table 4: Evaluation times of the Helmholtz free energy function and its gradient (Figure 5). Times are given relative to that of the original function with both (1) n=1 and (2) n corresponding to each column. (For instance, reverse mode AD with n=43 takes approximately twice the time to evaluate relative to the original function with n=43.) Times are measured by averaging a thousand runs on a machine with Intel Core i7-4785T 2.20 GHz CPU and 16 GB RAM, using DiffSharp 0.5.7. The evaluation time for the original function with n=1 is 0.0023 ms.

	n, number of variables							
	1	8	15	22	29	36	43	50
f, original								
Rel. $n=1$	1	5.12	14.51	29.11	52.58	84.00	127.33	174.44
∇f , numerical diff.								
Rel. $n=1$	1.08	35.55	176.79	499.43	1045.29	1986.70	3269.36	4995.96
Rel. n in column	1.08	6.93	12.17	17.15	19.87	23.64	25.67	28.63
∇f , forward AD								
Rel. $n=1$	1.34	13.69	51.54	132.33	251.32	469.84	815.55	1342.07
Rel. n in column	1.34	2.66	3.55	4.54	4.77	5.59	6.40	7.69
∇f , reverse AD								
Rel. $n=1$	1.52	11.12	31.37	67.27	113.99	174.62	254.15	342.33
Rel. n in column	1.52	2.16	2.16	2.31	2.16	2.07	1.99	1.96

Second-order methods based on Newton's method make use of both the gradient ∇f and the Hessian \mathbf{H}_f , working via updates of the form $\Delta \mathbf{w} = -\eta \mathbf{H}_f^{-1} \nabla f$ and providing significantly faster convergence (Press et al., 2007). AD provides a way of automatically computing the exact Hessian, enabling succinct and convenient general-purpose implementations. Newton's method converges in fewer iterations, but this comes at the cost of having to compute \mathbf{H}_f in each iteration. In large-scale problems, the Hessian is usually replaced by a numerical approximation using first-order updates from gradient evaluations, giving rise to quasi-Newton methods. A highly popular such method is the BFGS¹⁶ algorithm, together with its limited-memory variant L-BFGS (Dennis and Schnabel, 1996). On the other hand, Hessians arising in large-scale applications are typically sparse. This sparsity, along with symmetry, can be readily exploited by AD techniques such as computational graph elimination (Dixon, 1991), partial separability (Gay, 1996), and matrix coloring and compression (Gebremedhin et al., 2009).

In many cases one does not need the full Hessian but only a Hessian–vector product $\mathbf{H}\mathbf{v}$, which can be computed efficiently using a reverse-on-forward configuration of AD by applying the reverse mode to take the gradient of code produced by the forward mode. Given the function $f: \mathbb{R}^n \to \mathbb{R}$, the evaluation point \mathbf{x} , and the vector \mathbf{v} , one can accomplish this by first computing the directional derivative $\nabla f \cdot \mathbf{v}$ through the forward mode via setting $\dot{\mathbf{x}} = \mathbf{v}$ and then applying the reverse mode on this result to get $\nabla^2 f \cdot \mathbf{v} = \mathbf{H}_f \mathbf{v}$ (Pearlmutter, 1994). This computes $\mathbf{H}\mathbf{v}$ with O(n) complexity, even though \mathbf{H} is a $n \times n$ matrix.

Another approach for improving the rate of convergence of gradient methods is to use gain adaptation methods such as stochastic meta-descent (SMD) (Schraudolph, 1999), where stochastic sampling is introduced to avoid local minima and reduce the computational expense. An example using SMD with AD Hessian–vector products is given by Vishwanathan et al. (2006) on conditional random fields (CRF), a probabilistic method for labeling and segmenting data. Similarly, Schraudolph and Graepel (2003) use Hessian–vector products in their model combining conjugate gradient techniques with stochastic gradient descent.

4.2 Neural Networks and Deep Learning

Training of neural networks is an optimization problem with respect to the set of weights, which can in principle be addressed using any method including gradient descent, stochastic gradient descent (Bottou, 2010), or BFGS (Apostolopoulou et al., 2009). As we have seen, the backpropagation algorithm is only a special case of reverse mode AD: by applying AD to any objective function evaluating a network's error as a function of its weights, we can readily compute the partial derivatives needed for performing weight updates.¹⁷

Prevailing machine learning frameworks increasingly provide differentiation capability in one way or another; however, the underlying mechanism is not always made clear and confusion abounds regarding the use of the terms "autodiff", "automatic differentiation", and "symbolic differentiation", which are sometimes even used interchangeably. Main-

^{15.} See http://gbaydin.github.io/DiffSharp/examples-newtonsmethod.html for an implementation of Newton's method with the full Hessian.

^{16.} After Broyden-Fletcher-Goldfarb-Shanno, who independently discovered the method in the 1970s.

See http://gbaydin.github.io/DiffSharp/examples-neuralnetworks.html for an implementation of backpropagation with reverse mode AD.

stream frameworks including Theano¹⁸ (Bastien et al., 2012), TensorFlow (Abadi et al., 2016), Caffe (Jia et al., 2014), and CNTK (Seide and Agarwal, 2016) require the users to define static computation graphs within the syntactic and semantic constraints of a domain-specific mini language with limited support for control flow, whereas the lineage of projects leading from autograd¹⁹ and torch-autograd²⁰ to PyTorch²¹ provide truly general-purpose reverse mode AD capability of the type we outline in Section 3.

There are instances in neural network literature—albeit few—where explicit reference is made to AD for computing error gradients, such as Eriksson et al. (1998) using AD for large-scale feed-forward networks, and the work by Yang et al. (2008), where they use AD to train a neural network-based proportional-integral-derivative (PID) controller. Similarly, Rollins (2009) uses reverse mode AD in conjunction with neural networks for the problem of optimal feedback control.

Beyond backpropagation, the generality of AD also opens up other possibilities. An example is given for continuous time recurrent neural networks (CTRNN) by Al Seyab and Cao (2008), where they apply AD for the training of CTRNNs predicting dynamic behavior of nonlinear processes in real time. The authors use AD for computing derivatives higher than second-order and report significantly reduced network training time compared with other methods.

4.3 Computer Vision and Image Processing

In image processing, first- and second-order derivatives play an important role in tasks such as edge detection and sharpening (Russ, 2010). However, in most applications, these fundamental operations are applied on discrete functions of integer image coordinates, approximating those derived on a hypothetical continuous image space. As a consequence, derivatives are approximated using numerical differences.

On the other hand, many problems in computer vision are formulated as the minimization of an appropriate energy functional (Bertero et al., 1988; Chambolle, 2000). This minimization is usually accomplished via calculus of variations and the Euler-Lagrange equation. Pock et al. (2007) introduce AD to computer vision, addressing the problems of denoising, segmentation, and recovery of information from stereoscopic image pairs, and noting the usefulness of AD in identifying sparsity patterns in large Jacobian and Hessian matrices. In another study, Grabner et al. (2008) use reverse mode AD for GPU-accelerated medical 2D/3D registration, a task involving the alignment of data from different sources such as X-ray images or computed tomography. The authors report a six-fold increase in speed compared with numerical differentiation using center difference (cf. our benchmark with the Helmholtz function, Figure 5 and Table 4). Barrett and Siskind (2013) present a use of general-purpose AD for the task of video event detection. Compared with general computer vision tasks focused on recognizing objects and their properties (which can be

^{18.} Theano is a computational graph optimizer and compiler with GPU support and it currently handles derivatives in a highly optimized form of symbolic differentiation. The result can be interpreted as a hybrid of symbolic differentiation and reverse mode AD, but Theano does not use the reverse AD technique as we describe in this article. (Personal communication with the authors.)

^{19.} https://github.com/HIPS/autograd

^{20.} https://github.com/twitter/torch-autograd

^{21.} http://pytorch.org/

thought of as *nouns* in a narrative), an important aspect of this work is that it aims to recognize and reason about events and actions (i.e., *verbs*). The method uses Hidden Markov Models (HMMs) and Dalal and Triggs (2005) object detectors, and performs training on a corpus of pre-tracked video by an adaptive step size naïve gradient descent algorithm, where gradient computations are done with reverse mode AD. Initially implemented with the R6RS-AD package²² which provides forward and reverse mode AD in R6RS Scheme, the gradient code was later ported to C and highly optimized. Even if the final detection code does not directly use AD, the authors report²³ that AD in this case served as a foundation and a correctness measure for validating subsequent work.

4.4 Natural Language Processing

Natural language processing (NLP) constitutes one of the areas where rapid progress is being made by applying deep learning techniques (Collobert and Weston, 2008), exemplified by recent advances in neural machine translation (Bahdanau et al., 2014). Besides deep learning, statistical models in NLP are commonly trained using general purpose or specialized gradient-based methods and mostly remain expensive to train. Improvements in training time can be realized by using online or distributed training algorithms (Gimpel et al., 2010). An example using stochastic gradient descent for NLP is given by Finkel et al. (2008) optimizing conditional random field parsers through an objective function. Related with the work on video event detection in the previous section, Yu and Siskind (2013) report their work on sentence tracking, representing an instance of grounded language learning paired with computer vision, where the system learns word meanings from short video clips paired with descriptive sentences. The method uses HMMs to represent changes in video frames and meanings of different parts of speech. This work is implemented in C and computes the required gradients using AD through the ADOL-C tool.²⁴

4.5 Probabilistic Modeling and Inference

Inference techniques in probabilistic programming (Goodman, 2013) can be static, such as compiling a given model to Bayesian networks and using algorithms such as belief propagation for inference; or they can be dynamic, executing a model forward many times and computing statistics on observed values to infer distributions. Markov chain Monte Carlo (MCMC) (Neal, 1993) methods are often used for dynamic inference, such as the Metropolis–Hastings algorithm based on random sampling (Chib and Greenberg, 1995). Meyer et al. (2003) give an example of how AD can be used to speed up Bayesian posterior inference in MCMC, with an application in stochastic volatility.

When model parameters are continuous, the Hamiltonian—or, hybrid—Monte Carlo (HMC) algorithm provides improved convergence characteristics avoiding the slow exploration of random sampling, by simulating Hamiltonian dynamics through auxiliary "momentum variables" (Duane et al., 1987). The advantages of HMC come at the cost of requiring gradient evaluations of complicated probability models. AD is highly suitable

^{22.} https://github.com/qobi/R6RS-AD

^{23.} Personal communication.

^{24.} An implementation of the sentence tracker applied to video search using sentence-based queries can be accessed online: http://upplysingaoflun.ecn.purdue.edu/~qobi/cccp/sentence-tracker-video-retrieval.html

here for complementing probabilistic modeling, because it relieves the user from the manual derivation of the gradients for each model. For instance, the probabilistic programming language Stan (Carpenter et al., 2016) implements automatic Bayesian inference based on HMC and the No-U-Turn sampler (NUTS) (Hoffman and Gelman, 2014) and uses reverse mode AD for the calculation of gradients for both HMC and NUTS (Carpenter et al., 2015). Similarly, Wingate et al. (2011) demonstrate the use of AD as a nonstandard interpretation of probabilistic programs enabling efficient inference algorithms and Kucukelbir et al. (2017) present an AD-based method for deriving variational inference algorithms.

5. Implementations

It is useful to have an understanding of the different ways in which AD can be implemented. Here we cover major implementation strategies and provide a survey of existing tools.

A principal consideration in any AD implementation is the performance overhead introduced by the AD arithmetic and bookkeeping. In terms of computational complexity, AD ensures that the amount of arithmetic goes up by no more than a small constant (Griewank and Walther, 2008). But, managing this arithmetic can introduce a significant overhead if done carelessly. For instance, naïvely allocating data structures for holding dual numbers will involve memory access and allocation for every arithmetic operation, which are usually more expensive than arithmetic operations on modern computers. Likewise, using operator overloading may introduce method dispatches with attendant costs, which, compared to raw numerical computation of the original function, can easily amount to a slowdown of an order of magnitude.

Another major issue is the possibility of a class of bugs called "perturbation confusion" (Siskind and Pearlmutter, 2005). This essentially means that if two ongoing differentiations affect the same piece of code, the two formal epsilons they introduce (Section 3.1.1) need to be kept distinct. It is very easy to have bugs—particularly in performance-oriented AD implementations—that confuse these in various ways. Such situations can also arise when AD is nested, that is, derivatives are computed for functions that internally take derivatives.

One should also be cautious about approximated functions and AD. In this case, if you have a procedure approximating an ideal function, AD always gives the derivative of the procedure that was actually programmed, which may not be a good approximation of the derivative of the ideal function that the procedure was approximating. For instance, consider e^x computed by a piecewise-rational approximation routine. Using AD on this routine would produce an approximated derivative in which each piece of the piecewise formula will get differentiated. Even if this would remain an approximation of the derivative of e^x , we know that $\frac{de^x}{dx} = e^x$ and the original approximation itself was already a better approximation for the derivative of e^x . Users of AD implementations must be therefore cautious to approximate the derivative, not differentiate the approximation. This would require explicitly approximating a known derivative, in cases where a mathematical function can only be computed approximately but has a well-defined mathematical derivative.

In Table 5 we present a review of notable general-purpose AD implementations.²⁶ A thorough taxonomy of implementation techniques was introduced by Juedes (1991), which

^{25.} In modern systems this is not an issue, because e^x is a primitive implemented in hardware.

^{26.} Also see the website http://www.autodiff.org/ for a list of tools maintained by the AD community.

was later revisited by Bischof et al. (2008) and simplified into elemental, operator overloading, compiler-based, and hybrid methods. We adopt a similar classification for the following part of this section.

5.1 Elemental Libraries

These implementations form the most basic category and work by replacing mathematical operations with calls to an AD-enabled library. Methods exposed by the library are then used in function definitions, meaning that the decomposition of any function into elementary operations is done manually when writing the code.

The approach has been utilized since the early days of AD, prototypical examples being the WCOMP and UCOMP packages of Lawson (1971), the APL package of Neidinger (1989), and the work by Hinkins (1994). Likewise, Rich and Hill (1992) formulate their implementation of AD in MATLAB using elemental methods.

Elemental methods still constitute the simplest strategy to implement AD for languages without operator loading.

5.2 Compilers and Source Code Transformation

These implementations provide extensions to programming languages that automate the decomposition of equations into AD-enabled elementary operations. They are typically executed as preprocessors²⁷ to transform the input in the extended language into the original language.

Classical instances of source code transformation include the Fortran preprocessors GRESS (Horwedel et al., 1988) and PADRE2 (Kubo and Iri, 1990), which transform ADenabled variants of Fortran into standard Fortran 77 before compiling. Similarly, the ADIFOR tool (Bischof et al., 1996), given a Fortran source code, generates an augmented code in which all specified partial derivatives are computed in addition to the original result. For procedures coded in ANSI C, the ADIC tool (Bischof et al., 1997) implements AD as a source transformation after the specification of dependent and independent variables. A recent and popular tool also utilizing this approach is Tapenade (Pascual and Hascoët, 2008; Hascoët and Pascual, 2013), implementing forward and reverse mode AD for Fortran and C programs. Tapenade itself is implemented in Java and can be run locally or as an online service. ²⁸

In addition to language extensions through source code transformation, there are implementations introducing new languages with tightly integrated AD capabilities through special-purpose compilers or interpreters. Some of the earliest AD tools such as SLANG (Adamson and Winant, 1969) and PROSE (Pfeiffer, 1987) belong to this category. The NAGWare Fortran 95 compiler (Naumann and Riehme, 2005) is a more recent example, where the use of AD-related extensions triggers automatic generation of derivative code at compile time.

As an example of interpreter-based implementation, the algebraic modeling language AMPL (Fourer et al., 2002) enables objectives and constraints to be expressed in mathematical notation, from which the system deduces active variables and arranges the nec-

^{27.} Preprocessors transform program source code before it is given as an input to a compiler.

^{28.} http://www-tapenade.inria.fr:8080/tapenade/index.jsp

Table 5: Survey of major AD implementations.

Language	Tool	Type	Mode	e Institution / Project	References	URL
AMPL C, C++	AMPL ADIC	INT ST	F, R F, R	Bell Laboratories Argonne National Laboratory	Fourer et al. (2002) Bischof et al. (1997)	http://www.ampl.com/ http://www-new.mcs.anl.gov/adic/down-2.htm
C++	ADOL-C Ceres Solver	OO LIB	F, R F	Computational Infrastructure for Operations Research Google	Walther and Griewank (2012)	http://www.coin-or.org/projects/ADOL-C.xml http://ceres-solver.org/
C#	CppAD FADBAD++ Mxyzptlk AutoDiff	00 - 00 00 LIB	F, R F, R F R	Computational Infrastructure for Operations Research Technical University of Denmark Fermi National Accelerator Laboratory George Mason Univ., Department of Computer Science	Bell and Burke (2008) Bendtsen and Stauning (1996) Ostiguy and Michelotti (2007) Shtof et al. (2013)	http://www.coin-or.org/CppAD/ http://www.fadbad.com/fadbad.html https://cdcvs.fnal.gov/redmine/projects/fermitools/wiki/MXYZPTL http://autodiff.codeplex.com/
F# Fortran	DiffSharp ADIFOR NAGWare TAMC	OO ST COM ST	F, R F, R F, R R	National University of Ireland Maynooth Argonne National Laboratory Numerical Algorithms Group Max Planck Institute for Meteorology	Bischof et al. (1996) Naumann and Riehme (2005) Giering and Kaminski (1998)	http://diffsharp.github.io http://www.mcs.anl.gov/research/projects/adifor/ http://www.nag.co.uk/nagware/Research/ad_overyiew.asp http://autodiff.com/tamc/
Fortran, $C/C++$	COSY	INT	F	Michigan State Univ., Biomedical and Physical Sciences	Berz et al. (1996)	http://www.bt.pa.msu.edu/index_cosy.htm
Haskell Java	Tapenade ad Deriva	ST OO LIB	F, R F, R F	INRIA Sophia-Antipolis Haskell package Java & Clojure library	Hascoët and Pascual (2013)	http://www-sop.inria.fr/tropics/tapenade.html http://hackage.haskell.org/package/ad https://github.com/lambder/Deriva
MATLAB	B ADiMat INTLab	ST, OO OO	F, R F	Technical University of Darmstadt, Scientific Computing Hamburg University of Technology, Institute for Reli-	Willkomm and Vehreschild (2013) Rump (1999)	http://adimat.sc.informatik.tu-darmstadt.de/ http://www.ti3.tu-harburg.de/rump/intlab/
	TOMLAB /MAD	00	F	able Computing Cranfield University & Tomlab Optimization Inc.	Forth (2006)	http://tomlab.biz/products/mad
Python	ad	00	R	Python package		https://pypi.python.org/pypi/ad
Scheme	autograd R6RS-AD Scmutils	00 00	R F, R F	Harvard Intelligent Probabilistic Systems Group Purdue Univ., School of Electrical and Computer Eng. MIT Computer Science and Artificial Intelligence Lab.	Sussman and Wisdom (2001)	https://github.com/HIPS/autograd https://github.com/qobi/R6RS-AD http://groups.csail.mit.edu/mac/users/gjs/6946/refman.txt

F: Forward, R: Reverse; COM: Compiler, INT: Interpreter, LIB: Library, OO: Operator overloading, ST: Source transformation

essary AD computations. Other examples in this category include the FM/FAD package (Mazourik, 1991), based on the Algol-like DIFALG language, and the object-oriented COSY language (Berz et al., 1996) similar to Pascal.

The Stalingrad compiler (Pearlmutter and Siskind, 2008a; Siskind and Pearlmutter, 2008a), working on the Scheme-based AD-aware VLAD language, also falls under this category. The newer DVL compiler²⁹ is based on Stalingrad and uses a reimplementation of portions of the VLAD language.

5.3 Operator Overloading

In modern programming languages with polymorphic features, operator overloading provides the most straightforward way of implementing AD, exploiting the capability of redefining elementary operation semantics.

A popular tool implemented with operator overloading in C++ is ADOL-C (Walther and Griewank, 2012). ADOL-C requires the use of AD-enabled types for variables and records arithmetic operators on variables in data structures called "tapes", which can subsequently be "played back" during reverse mode AD computations. The Mxyzptlk package (Michelotti, 1990) is another example for C++ capable of computing arbitrary-order partial derivatives via forward propagation. The FADBAD++ library (Bendtsen and Stauning, 1996) implements AD for C++ using templates and operator overloading. For Python, the *ad* package³⁰ uses operator overloading to compute first- and second-order derivatives, while the newer *autograd* package³¹ uses reverse mode AD with support for higher-order derivatives.

For functional languages, examples include R6RS-AD³² and the AD routines within the Scmutils library³³ for Scheme, the ad library³⁴ for Haskell, and the DiffSharp library³⁵ for F#.

6. Conclusions

We have shown that using AD in machine learning enables one to build models using the full expressivity of general-purpose programming languages, knowing that any needed derivatives can be evaluated accurately and efficiently without any additional coding effort. Needless to say, there are occasions where one can be interested in obtaining more than just the numerical value of derivatives. Derivative expressions can be useful for mathematical analysis and offer valuable insight into the problem domain. However, for any non-trivial function of more than a handful of variables, analytic expressions for gradients or Hessians increase so rapidly in complexity as to render any interpretation unlikely.

An important direction for future work is to make use of nested AD techniques in machine learning, allowing differentiation to be nested arbitrarily deep with referential transparency (Siskind and Pearlmutter, 2008b; Pearlmutter and Siskind, 2008b). Nested AD is

^{29.} https://github.com/axch/dysvunctional-language

^{30.} http://pythonhosted.org/ad/

^{31.} https://github.com/HIPS/autograd

 $^{32.\ \}text{https://github.com/NUIM-BCL/R6RS-AD}$

^{33.} http://groups.csail.mit.edu/mac/users/gjs/6946/refman.txt

^{34.} http://hackage.haskell.org/package/ad

^{35.} http://diffsharp.github.io

highly relevant in hyperparameter optimization as it can effortlessly provide exact hypergradients (Maclaurin et al., 2015; Baydin et al., 2017), that is, derivatives of a training objective with respect to the hyperparameters of an inner optimization routine. Potential applications include Bayesian model selection (Rasmussen and Williams, 2006) and gradient-based tuning of Hamiltonian Monte Carlo step sizes and mass-matrices (Salimans et al., 2015). Besides hyperparameters, models internally using higher-order derivatives constitute a straightforward usage case for nested AD. The Riemannian manifold Langevin and Hamiltonian Monte Carlo methods (Girolami and Calderhead, 2011) use higher-order derivative information to more closely track the information geometry of the sampled distribution for faster convergence and exploration. In neural networks, it is very natural to use nested derivatives in defining objective functions that take input transformations into account, such as the Tangent Prop method (Simard et al., 1998) for imposing invariance under a set of chosen transformations.

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