Automatic Differentiation

Ingo Blechschmidt

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1 What automatic differentiation achives

Given code which implements a function $x \mapsto f(x)$, automatic differentation gives us code which implements its derivative $x \mapsto f'(x)$. The code obtained this way is exactly the same as if we'd worked out the derivative on paper.

The input code to automatic differentiation may contain arbitrary control structures such as *if* conditionals or *while* loops. Therefore it is applicable to a wide range of problems:

- The basic use case is to find the derivative of a function.
- Assume that we're using Newton's method to solve a parameter-dependent equation $f(x, \theta) = 0$ for x. We might be interested in how the solution $x(\theta)$ depends on θ. This is trivial with automatic differentiation, we just feed it our Newton code.
- Assume that we're solving some parameter-dependent ordinary differential equation. We are interested in the dependence of the solution (at the final time, say) on the parameter. For this, we just hand our differential equation solving code to automatic differentiation.

Automatic differentiation is totally unlike *numerical differentiation*. With numerical differentiation, we approximate $f'(x)$ by some difference quotient like

$$\frac{f(x+h) - f(x)}{h} \qquad \text{or} \qquad \frac{f(x+h) - f(x-h)}{2h}.$$

This approach faces severe problems: If h is large, the quotient won't be a good approximation to the true derivative. Instead, it will give the slope of some unrelated secant. If h is small, the approximation will be good in theory. But practically, with floating-point arithmetic, a huge loss of precision may occur, since we are subtracting two nearly equal numbers.

Automatic differentiation is also unlike *symbolic differentiation*, which operates on the level of *terms*. Symbolic differentiation is useful if our goal is to obtain *formulas* for various quantities, but it isn't particularly suited for efficient evaluation to floating-point numbers.

2 The basic idea of automatic differentiation

To grasp the basic idea of automatic differentiation, assume that there exists a magical number ε such that $\varepsilon^2 = 0$. This number ε should not itself be zero, as else we couldn't extract any meaningful information from calculations with ε.

The set of real numbers doesn't contain such a number. Nevertheless, watch:

$$\begin{aligned}
(x+\varepsilon)^2 &= x^2 + 2x\varepsilon + \varepsilon^2 = x^2 + 2x\varepsilon \\
(x+\varepsilon)^3 &= x^2 + 3x^2\varepsilon + 3x\varepsilon^2 + \varepsilon^3 = x^3 + 3x^2\varepsilon \\
\frac{1}{x+\varepsilon} &= \frac{x-\varepsilon}{(x+\varepsilon)\cdot(x-\varepsilon)} = \frac{x-\varepsilon}{x^2} = \frac{1}{x} - \frac{1}{x^2}\varepsilon
\end{aligned}$$

So it appears that plugging in $x+\varepsilon$ into a function f yields *the derivative* $f'(x)$ *along with the function value* $f(x)$, as the coefficient of the magical number ε.

We exploit this observation with automatic differentiation. To calculate the derivative $f'(x)$, given code for $f(x)$, we feed the code with $x+\varepsilon$ and then extract the coefficient of ε from the result. Of course, the given code didn't expect to be called with magical ε's instead of ordinary floating-point numbers. But in a language with operator overloading, there's no way for the code to prevent such unusual evaluations. We discuss this in more detail below.

3 A closer look: the dual numbers

Recall how we construct the complex numbers $\mathbb{C}$ from the real numbers $\mathbb{R}$. We define $\mathbb{C} := \mathbb{R} \times \mathbb{R}$ and set

$$\begin{aligned}
(x,a) + (y,b) &:= (x+y, a+b), \\
(x,a) \cdot (y,b) &:= (xy - ab, xb + ay).
\end{aligned}$$

These formulas don't appear from nowhere. Instead, setting $i := (0,1)$, they are precisely the formulas needed such that the identity $i^2 = -1$ holds. Writing $(x,a) = x + ai$, we call x the *real part* and a the *imaginary part*.

In a similar way, we can construct the *dual numbers* $\mathbb{R}[\varepsilon]/(\varepsilon^2)$. We define $\mathbb{R}[\varepsilon]/(\varepsilon^2) := \mathbb{R}\times\mathbb{R}$ and set

$$\begin{aligned}
(x,a) + (y,b) &:= (x+y, a+b), \\
(x,a) \cdot (y,b) &:= (xy, xb + ay).
\end{aligned}$$

Again, these formulas can be motivated. We write $\varepsilon := (0,1)$ and $x + a\varepsilon := (x,a)$. Then these rules can be obtained by formally expanding $(x+a\varepsilon)+(y+b\varepsilon)$ respectively $(x+a\varepsilon)\cdot(y+b\varepsilon)$ and imposing the relation $\varepsilon^2 = 0$.

It's easy to implement a data type of dual numbers in languages such as Haskell or Python.

```
-- Haskell
data D a = D a a deriving (Show,Eq)

instance (Num a) => Num (D a) where
    D x a + D y b  = D (x + y)          (a + b)
    D x a * D y b  = D (x * y)          (x * b + a * y)
    negate (D x a) = D (negate x)       (negate a)
    fromInteger n  = D (fromInteger n) 0
```

If `f` is a function `(Num a) => a -> a`, then evaluating `f (D x 1)` will yield `D (f x) (f' x)`. A live example in the interactive Haskell shell looks like this:

```
> let f x = x^2
> f (D 5 1)
D 25 10
```

We can also define a higher-order function which takes a function and returns its derivative:

```
> let diff f x = b where D y b = f (D x 1)
> diff f 5
10
```

```
# Python
class Dual(object):
    def __init__(self, x, a):
        self.x = x
        self.a = a

    def __add__(self, other):
        return Dual(self.x + other.x, self.a + other.a)

    def __mul__(self, other):
        return Dual(self.x * other.x,
                    other.x * self.a + self.x * other.a)
```

```
>>> def f(x): return x*x
>>> f(Dual(5,1)).x
25
>>> f(Dual(5,1)).a
10
```

4 Why automatic differentiation works

Taylor expansion gives a slick proof that automatic differentiation works for polynomials. Recall that if f is a polynomial, we have the identity

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2!}f''(x)h^2 + \frac{1}{3!}f'''(x)h^3 + \cdots .$$

The sum on the right only looks like an infinite sum. In fact, it terminates with the term containing $h^{\deg(f)}$ being the last one. This identity is purely algebraic; no convergence considerations are necessary. Therefore it's plausible, and in fact easy to prove, that this form of Taylor expansion holds over any kind of numbers – the real numbers, the complex numbers, and the dual numbers. Plugging in $h := \varepsilon$, we obtain

$$f(x+\varepsilon) = f(x) + f'(x)\varepsilon,$$

with all further terms dropping out because $\varepsilon^2 = \varepsilon^3 = \cdots = 0$. This is the reason why automatic differentiation works on polynomials.

For the general case we prove the following theorem: If a function f is built from other functions using addition, multiplication, and composition, and if automatic differentiation works for the constituent functions, then it also works for f.

To this end, define the *lift* of a differentiable function $f : \mathbb{R} \to \mathbb{R}$ to be the function

$$\overline{f} : \mathbb{R}[\varepsilon]/(\varepsilon^2) \to \mathbb{R}[\varepsilon]/(\varepsilon^2),\ x + a\varepsilon \mapsto f(x) + f'(x)a\varepsilon.$$

A precise statement of the theorem is then: Let $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$ be differentiable functions. Then

$$\overline{f+g} = \overline{f} + \overline{g}, \quad \overline{f \cdot g} = \overline{f} \cdot \overline{g}, \quad \overline{f \circ g} = \overline{f} \circ \overline{g}.$$

For fun, we verify the case for multiplication and composition:

$$\begin{aligned}
(\overline{f} \cdot \overline{g})(x + a\varepsilon) &= \overline{f}(x + a\varepsilon) \cdot \overline{g}(x + a\varepsilon) \\
&= (f(x) + f'(x)a\varepsilon) \cdot (g(x) + g'(x)a\varepsilon)c \\
&= f(x)g(x) + (f(x)g'(x) + f'(x)g(x))a\varepsilon \\
&= \overline{f \cdot g}(x + a\varepsilon)
\end{aligned}$$

$$\begin{aligned}
(\overline{f} \circ \overline{g})(x + a\varepsilon) &= \overline{f}(\overline{g}(x + a\varepsilon)) \\
&= \overline{f}(g(x) + g'(x)a\varepsilon) \\
&= f(g(x)) + f'(g(x))g'(x)a\varepsilon \\
&= \overline{f \circ g}(x + a\varepsilon)
\end{aligned}$$

In numerical practice, code for evaluating a function may well be huge and complex. However, it is composed of elementary functions (like sine and cosine) and addition, multiplication, and composition. If the library for automatic differentiation correctly implements the elementary functions, any composite function will be correctly derived as well.

5 Caveats and outlook

Higher order Automatic differentiation can be easily extended to calculate higher derivatives as well. For instance, employing a magical number ε such that $\varepsilon^3 = 0$, we have for polynomials

$$f(x+\varepsilon) = f(x) + f'(x)\varepsilon + \frac{1}{2!}f''(x)\varepsilon^2.$$

We could also simply use nested dual numbers.

Higher dimensions Automatic differentiation can also be extended to multiple dependent or independent variables. The procedure described here is called *forward-mode automatic differentiation*, which is efficient for functions $\mathbb{R} \to \mathbb{R}^n$. There is also a variant called *backward-mode automatic differentiation*, which is efficient for functions $\mathbb{R}^n \to \mathbb{R}$.

Fun fact: Using backward-mode automatic differentiation on code for evaluating a neural network ("feedforward") automatically gives code for the standard backpropagation algorithm.

Poor man's automatic differentiation Stuck with a language without operator overloading? And you don't feel like using one of the time-tested code-transformation packages, which are available even for Fortran? Then check whether the following variant of automatic differentiation is good enough for you. Its idea is to employ the standard imaginary unit i instead of ε as magical number: Approximate $f'(x)$ by

$$f'(x) \approx \operatorname{Im} \frac{f(x+hi)}{h}$$

with h small. Since Taylor expansion yields

$$f(x+hi) = f(x) + f'(x)hi - \frac{1}{2!}f''(x)h^2 - \frac{1}{3!}f'''(x)h^3 i + \cdots,$$

the imaginary part of $f(x+hi)/h$ is

$$f'(x) - \frac{1}{3!}f'''(x)h^2 + h^4 \cdot (\cdots),$$

which might be a good approximation to $f'(x)$ if h is sufficiently small.

```
> import Data.Complex
> sin (0 :+ 0.001) / 0.001  -- the correct derivative is 1.0
0.0 :+ 1.0000001666666751
```

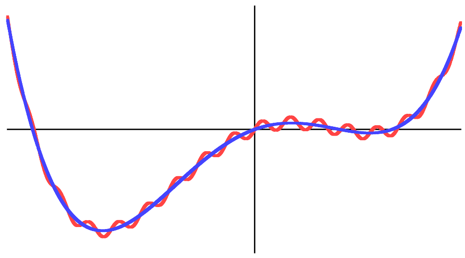
Points of non-differentiability Consider the absolute value function with its point of non-differentiability. How should $|x + a\varepsilon|$ be defined? Of course, for positive x it should be $x + a\varepsilon$ and for negative x it should be $-x - a\varepsilon$. But for $x = 0$ there is no sensible definition of $|x + a\varepsilon|$. An implementation either has to throw an error in this case or return a fictional value such as 0 or `NaN`.

The problem is exacerbated by terms like $\sqrt{x^4}$. This term is infinitely differentiable, even in the point $x = 0$. However, the chain rule cannot be used evaluate the derivative. Automatic differentiation as a kind of glorified chain rule will therefore not work correctly either. Without a symbolic approach it's not possible to automatically simplify the expression to $\sqrt{x^4} = x^2$; also, this kind of simplification will not work with more complex expressions such as $\sqrt{x^4 + y^4}$.

Luckily, this problem doesn't seem to surface often. One explanation is that non-differentiability often occurs at isolated points. Precisely hitting those points with floating-point operations is hard. Secondly, many numerical algorithms don't use non-differentiable functions such as absolute value and square root in problematic places – for instance, Newton's method for solving nonlinear equations and all the familiar methods for solving ordinary differential equations don't.

Consistency error Applied to code which would (in the absence of rounding errors) exactly compute a function f, automatic differentiation will result in code which exactly computes its derivative f' (again in the absence of rounding errors). However, sometimes our code only calculates an approximation of the correct value – even if there were no rounding errors. For instance, this is the case when solving ordinary differential equations with Euler's method or some more sophisticated method.

Automatic differentiation will then produce code which gives the exact derivative of our approximated value, but not of the correct theoretical value. As a concrete example, consider the function f given by the blue curve in the following plot.



Assume that our code for evaluating f actually evaluates the function given by the red curve. If we are only interested in the function values, we might be content with this approximation. However, automatic differentiation would yield the derivative of the red curve, which is far off from the derivative of f. One could describe such a situation as "discretize first, then derive" instead of "derive first, then discretize".

Fortunately, this kind of pathology doesn't seem to occur often in real world problems. Give it a try!

Synthetic differential geometry Do you want to employ infinitesimal numbers like ε not only in your numerical algorithms, but also in your theoretical mathematical research? Do you want to freely use ε's as the physicists do? There is a way to do that, while at the same time staying mathematically rigorous. Check out an expository blog post by Andrej Bauer

`http://math.andrej.com/2008/08/13/intuitionistic-mathematics-for-physics/comment-page-1/`

or these notes for high school students (in German):

`https://github.com/iblech/mathezirkel-kurs/raw/master/thema05-sdg/blatt05.pdf`