Differentiate Automatically

VLC = Vision Learning Control

An Introduction to Automatic Differentiation

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Much of this material is based on this blog post:
`https://rufflewind.com/2016-12-30/reverse-mode-automatic-differentiation`

What is Automatic Differentiation (AD)?

To solve optimisation problems using gradient methods we need to compute the gradients (derivatives) of the objective with respect to the parameters.

- In neural nets we're talking about the gradients of the loss function, $\mathcal{L}$ with respect to the parameters $\boldsymbol{\theta}$: $\nabla_{\boldsymbol{\theta}}\mathcal{L} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}}$
- AD is important - it's been suggested that "Differentiable programming" could be the term that ultimately replaces deep learning[1].

[1] `http://forums.fast.ai/t/differentiable-programming-is-this-why-we-switched-to-pytorch/9589/5`

What is Automatic Differentiation (AD)?

Computing Derivatives

There are three ways to compute derivatives:

- Symbolically differentiate the function with respect to its parameters
  - by hand
  - using a CAS
- Make estimates using finite differences
- Use Automatic Differentiation

Problems

Static - can't "differentiate algorithms"

Problems

Numerical errors - will compound in deep nets

What is Automatic Differentiation (AD)?

Automatic Differentiation is:

- a method to get exact derivatives efficiently, by storing information as you go forward that you can reuse as you go backwards.
  - Takes code that computes a function and uses that to compute the derivative of that function.
  - The goal isn't to obtain closed-form solutions, but to be able to write a program that efficiently computes the derivatives.

Lets think about differentiation and programming

Example (Math)

$$x = ?$$
$$y = ?$$
$$a = x\,y$$
$$b = \sin(x)$$
$$z = a + b$$

Example (Code)

```
x = ?
y = ?
a = x * y
b = sin(x)
z = a + b
```

The Chain Rule of Differentiation

Recall the chain rule for a variable/function z that depends on y which depends on x:

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

In general, the chain rule can be expressed as:

$$\frac{\partial w}{\partial t} = \sum_i^N \frac{\partial w}{\partial u_i}\frac{\partial u_i}{\partial t} = \frac{\partial w}{\partial u_1}\frac{\partial u_1}{\partial t} + \frac{\partial w}{\partial u_2}\frac{\partial u_2}{\partial t} + \cdots + \frac{\partial w}{\partial u_N}\frac{\partial u_N}{\partial t}$$

where w is some output variable, and u_i denotes each input variable w depends on.

Applying the Chain Rule

Let's differentiate our previous expression with respect to some yet to be given variable t:

Expression

$x = ?$

$y = ?$

$a = x\,y$

$b = \sin(x)$

$z = a + b$

$$\frac{\partial x}{\partial t} = ?$$
$$\frac{\partial y}{\partial t} = ?$$
$$\frac{\partial a}{\partial t} = x\frac{\partial y}{\partial t} + y\frac{\partial x}{\partial t}$$
$$\frac{\partial b}{\partial t} = \cos(x)\frac{\partial x}{\partial t}$$
$$\frac{\partial z}{\partial t} = \frac{\partial a}{\partial t} + \frac{\partial b}{\partial t}$$

If we substitute $t = x$ in the above we'll have an algorithm for computing $\partial z/\partial x$. To get $\partial z/\partial y$ we'd just substitute $t = y$.

Translating to code I

We could translate the previous expressions back into a program involving *differential variables* `{dx, dy, ...}` which represent $\partial x/\partial t, \partial y/\partial t, \ldots$ respectively:

```
dx = ?
dy = ?
da = y * dx + x * dy
db = cos(x) * dx
dz = da + db
```

What happens to this program if we substitute $t = x$ into the math expression?

Translating to code II

```
dx = 1
dy = 0
da = y * dx + x * dy
db = cos(x) * dx
dz = da + db
```

The effect is remarkably simple: to compute $\partial z/\partial x$ we just seed the algorithm with `dx=1` and `dy=0`.

Translating to code III

```
dx = 0
dy = 1
da = y * dx + x * dy
db = cos(x) * dx
dz = da + db
```

To compute $\partial z/\partial y$ we just seed the algorithm with `dx=0` and `dy=1`.

Making Rules

- We've successfully computed the gradients for a specific function, but the process was far from automatic.
- We need to formalise a set of rules for translating a program that evaluates an expression into a program that evaluates its derivatives.
- We have actually already discovered 3 of these rules:

```
c = a + b    =>  dc = da + db
c = a * b    =>  dc = b * da + a * db
c = sin(a)   =>  dc = cos(a) * da
```

More rules

These initial rules:

```
c=a+b      =>   dc=da+db
c=a*b      =>   dc=b*da+a*db
c=sin(a)   =>   dc=cos(a)*da
```

can easily be extended further using multivariable calculus:

```
c=a-b      =>   dc=da-db
c=a/b      =>   dc=da/b-a*db/b**2
c=a**b     =>   dc=b*a**(b-1)*da+log(a)*a**b*db
c=cos(a)   =>   dc=-sin(a)*da
c=tan(a)   =>   dc=da/cos(a)**2
```


Forward Mode AD

- To translate using the rules we simply replace each primitive operation in the original program by its differential analogue.
- The order of computation remains unchanged: if a statement K is evaluated before another statement L, then the differential analogue of K is evaluated before the analogue statement of L.
- This is **Forward-mode Automatic Differentiation**.

Interleaving differential computation

A careful analysis of our original program and its differential analogue shows that its possible to interleave the differential calculations with the original ones:

```
x  = ?
dx = ?

y  = ?
dy = ?

a  = x * y
da = y * dx + x * dy

b  = sin(x)
db = cos(x) * dx

z  = a + b
dz = da + db
```

Dual Numbers

- This implies that we can keep track of the value and gradient at the same time.
- We can use a mathematical concept called a "Dual Number" to create a very simple direct implementation of AD.

Reverse Mode AD

- Whilst Forward-mode AD is easy to implement, it comes with a very big disadvantage...
- **For every variable we wish to compute the gradient with respect to, we have to run the *complete program* again.**
- This is obviously going to be a problem if we're talking about the gradients of a function with very many parameters (e.g. a deep network).
- A solution is **Reverse Mode Automatic Differentiation**.

Reversing the Chain Rule

The chain rule is symmetric — this means we can turn the derivatives upside-down:

$$\frac{\partial s}{\partial u} = \sum_i^N \frac{\partial w_i}{\partial u}\frac{\partial s}{\partial w_i} = \frac{\partial w_1}{\partial u}\frac{\partial s}{\partial w_1} + \frac{\partial w_2}{\partial u}\frac{\partial s}{\partial w_2} + \cdots + \frac{\partial w_N}{\partial u}\frac{\partial s}{\partial w_N}$$

In doing so, we have inverted the input-output role of the variables: u is some input variable, the w_i's are the output variables that depend on u. s is the yet-to-be-given variable.

In this form, the chain rule can be applied repeatedly to every input variable u (akin to how in forward mode we repeatedly applied it to every w). Therefore, given some s we expect this form of the rule to give us a program to compute both $\partial s/\partial x$ and $\partial s/\partial y$ in one go...

Reversing the chain rule: Example

$$\frac{\partial s}{\partial u} = \sum_i^N \frac{\partial w_i}{\partial u}\frac{\partial s}{\partial w_i}$$

$x = ?$
$y = ?$
$a = x\,y$
$b = \sin(x)$
$z = a + b$

$$\frac{\partial s}{\partial z} = ?$$

$$\frac{\partial s}{\partial b} = \frac{\partial z}{\partial b}\frac{\partial s}{\partial z} = \frac{\partial s}{\partial z}$$

$$\frac{\partial s}{\partial a} = \frac{\partial z}{\partial a}\frac{\partial s}{\partial z} = \frac{\partial s}{\partial z}$$

$$\frac{\partial s}{\partial y} = \frac{\partial a}{\partial y}\frac{\partial s}{\partial a} = x\frac{\partial s}{\partial a}$$

$$\frac{\partial s}{\partial x} = \frac{\partial a}{\partial x}\frac{\partial s}{\partial a} + \frac{\partial b}{\partial x}\frac{\partial s}{\partial b}$$

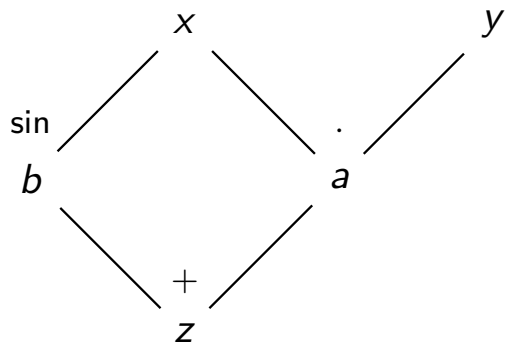
$$= y\frac{\partial s}{\partial a} + \cos(x)\frac{\partial s}{\partial b}$$

$$= (y + \cos(x))\frac{\partial s}{\partial z}$$

Visualising dependencies

Differentiating in reverse can be quite mind-bending: instead of asking what input variables an output depends on, we have to ask what output variables a given input variable can affect.

We can see this visually by drawing a dependency graph of the expression:



Translating to code

Let's now translate our derivatives into code. As before we replace the derivatives ($\partial s/\partial z, \partial s/\partial b, \ldots$) with variables (`gz`, `gb`, `...`) which we call *adjoint variables*:

```
gz = ?
gb = gz
ga = gz
gy = x * ga
gx = y * ga + cos(x) * gb
```

If we go back to the equations and substitute $s = z$ we would obtain the gradient in the last two equations. In the above program, this is equivalent to setting `gz = 1`.

This means to get the both gradients $\partial z/\partial x$ and $\partial z/\partial y$ we only need to run the program once!

Limitations of Reverse Mode AD

- If we have multiple output variables, we'd have to run the program for each one (with different seeds on the output variables)[2]. For example:

$$\begin{cases} z = 2x + \sin x \\ v = 4x + \cos x \end{cases}$$

- We can't just interleave the derivative calculations (since they all appear to be in reverse)... How can we make this automatic?

[2] there are ways to avoid this limitation...

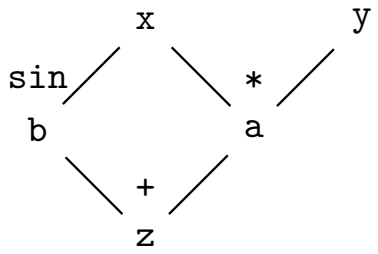
Implementing Reverse Mode AD

There are two ways to implement Reverse AD:

1. We can parse the original program and generate the *adjoint* program that calculates the derivatives.
   - Potentially hard to do.
   - Static, so can only be used to differentiate algorithms that have parameters predefined.
   - But, efficient (lots of opportunities for optimisation)
2. We can make a *dynamic* implementation by constructing a graph that represents the original expression as the program runs.

Constructing an expression graph

The goal is to get something akin to the graph we saw earlier:



The "roots" of the graph are the independent variables `x` and `y`. Constructing these nodes is as simple as creating an object:

```
class Var:
  def __init__(self, value):
    self.value = value
    self.children = []
    ...
  ...

x = Var(0.5)
y = Var(4.2)
```

Each `Var` node can have *children* which are the nodes that depend directly on that node. The children allow nodes to link together in a **Directed Acyclic Graph**.

Building expressions

By default, nodes do not have any children. As expressions are created each expression u registers itself as a child of each of its dependencies w_i together with its weight $\partial w_i / \partial u$ which will be used to compute gradients:

```
class Var:
  ...
  def __mul__(self, other):
    z = Var(self.value * other.value)

    # weight = dz/dself = other.value
    self.children.append((other.value, z))

    # weight = dz/dother = self.value
    other.children.append((self.value, z))
    return z
  ...
...
# "a" is a new Var that is a child of both x and y
a = x * y
```

Computing gradients

Finally, to get the gradients we need to propagate the derivatives. To avoid unnecessarily traversing the tree multiple times we will *cache* the derivative of a node in an attribute `grad_value`:

```
class Var:
  def __init__(self):
    ...
    self.grad_value = None

  def grad(self):
    if self.grad_value is None:
      # calculate derivative using chain rule
      self.grad_value = sum(weight * var.grad() for weight,
          var in self.children)
    return self.grad_value
        ...
...
a.grad_value = 1.0
print("da/dx = {}".format(x.grad()))
```


Aside: Optimising Reverse Mode AD

- The Reverse AD approach we've outlined is not very space efficient. One way to get around this is to avoid storing the children directly and instead store indices in an auxiliary data structure called a *Wengert list* or *tape*.
- Another interesting approach to memory reduction is trade-off computation for memory of the caches. The Count-Trailing-Zeros (CTZ) approach does just this[3].
- **But,** in reality memory is relatively cheap if managed well...

[3] Andreas Griewank (1992) Achieving logarithmic growth of temporal and spatial complexity in reverse automatic differentiation, Optimization Methods and Software, 1:1, 35-54, DOI: 10.1080/10556789208805505

AD in the PyTorch autograd package

- PyTorch's AD is remarkably similar to the one we've just built:
  - it eschews the use of a tape
  - it builds the computation graph as it runs (recording explicit `Function` objects as the children of `Tensors` rather than grouping everything into `Var` objects)
  - it caches the gradients in the same way we do (in the `grad` attribute) - hence the need to call `zero_grad()` when recomputing the gradients of the same graph after a round of backprop.
- PyTorch does some clever memory management to work well in a reference-counted regime and aggressively frees values that are no longer needed.
- The backend is actually mostly written in C++, so its fast, and can be multi-threaded (avoids problems of the GIL).
- It allows easy "turning off" of gradient computations through `requires_grad`.
- In-place operations which invalidate data needed to compute derivatives will cause runtime errors, as will variable aliasing...