Name:

CMSC 838B & 498Z: Differentiable Programming

Tues/Thur 12:30pm – 1:45pm
IRB 4105 (T) & IRB 5105 (R)
http://www.cs.umd.edu/class/fall2021/cmsc838b

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Why Automatic Differentiation (AD)?

To solve optimization problems using gradient methods we need to compute the gradients (derivatives) of the objective w.r.t. the parameters

- In neural nets we're talking about the gradients of the loss function w.r.t. the parameters $\boldsymbol{\theta}$: $\nabla L = \frac{\partial L}{\partial \theta}$
- AD is important - it's been suggested that "Differentiable programming" could be the term that ultimately replaces deep learning

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Computing Derivatives

Three ways to compute derivatives –

- **Symbolically differentiate the function w.r.t. its parameters**
  - **Problem**: Static - can't "differentiate algorithms"
- **Make estimates using finite differences**
  - Problems Problems: Numerical errors - will compound in deep nets
- **Use Automatic Differentiation**

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What is Automatic Differentiation (AD)

- 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.

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Differentiation and Programming

Example (Math)

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

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

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Applying the Chain Rule

- Let's differentiate the previous expression w.r.t. some yet to be given variable t:

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

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

- If we substitute t = x in the above we'll have an algorithm for computing dz/dx. To get dz/dy we'd just substitute t = y

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Translating to code I

We could translate the previous expressions back into a program involving differential variables {dx, dy, ...} which represent dx/dt, dy/dt, . . . 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?

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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 dz/dx we just seed the algorithm with dx=1 and dy=0.

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Translating to code III

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

To compute dz/dy we just seed the algorithm with dx=0 and dy=1

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Making Rules

- We've successfully computed the gradients for a specific function, but the process was far from automatic
- We need to formalize 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
```

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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=cos(a)    =>   dc=-sin(a)*da
c=tan(a)    =>   dc=da/cos(a)**2
```

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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**

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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 wi '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 ds/dx and ds/dy in one go. . .

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Reversing the Chain Rule: Example

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

$$\begin{aligned} x &= ? \\ y &= ? \\ a &= x\,y \\ b &= \sin(x) \\ z &= a + b \end{aligned}$$

$$\begin{aligned} \frac{\partial s}{\partial z} &= ? \\ \frac{\partial s}{\partial b} &= \frac{\partial z}{\partial b}\frac{\partial s}{\partial z} = \frac{\partial s}{\partial z} \\ \frac{\partial s}{\partial a} &= \frac{\partial z}{\partial a}\frac{\partial s}{\partial z} = \frac{\partial s}{\partial z} \\ \frac{\partial s}{\partial y} &= \frac{\partial a}{\partial y}\frac{\partial s}{\partial a} = x\,\frac{\partial s}{\partial a} \\ \frac{\partial s}{\partial x} &= \frac{\partial a}{\partial x}\frac{\partial s}{\partial a} + \frac{\partial b}{\partial x}\frac{\partial s}{\partial b} \\ &= y\,\frac{\partial s}{\partial a} + \cos(x)\,\frac{\partial s}{\partial b} \\ &= (y + \cos(x))\,\frac{\partial s}{\partial z} \end{aligned}$$

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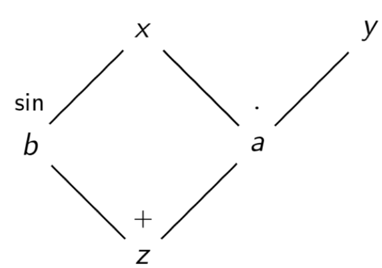
Visualizing Dependencies

- 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:



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Translating to Code

- Let's now translate our derivatives into code. As before we replace the derivatives (ds/dz, ds/db, . . .) 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 dz/dx and dz/dy we only need to run the program once!

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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). 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?

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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.

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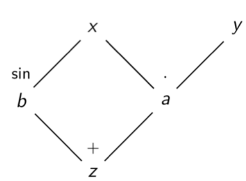
Constructing an Expression Graph

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.**

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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
```

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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 u= u {} ". format ( x. grad () )
```

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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

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