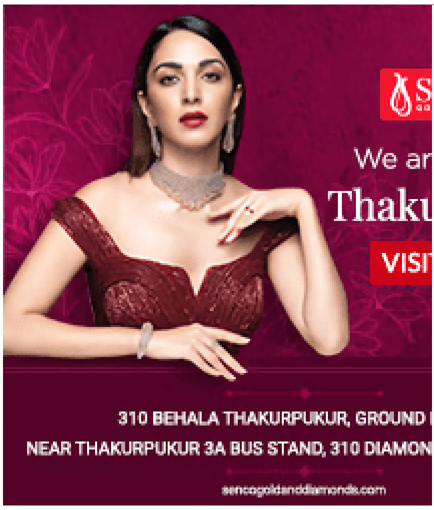
Programming Review



PyTorch | Automatic Differentiation

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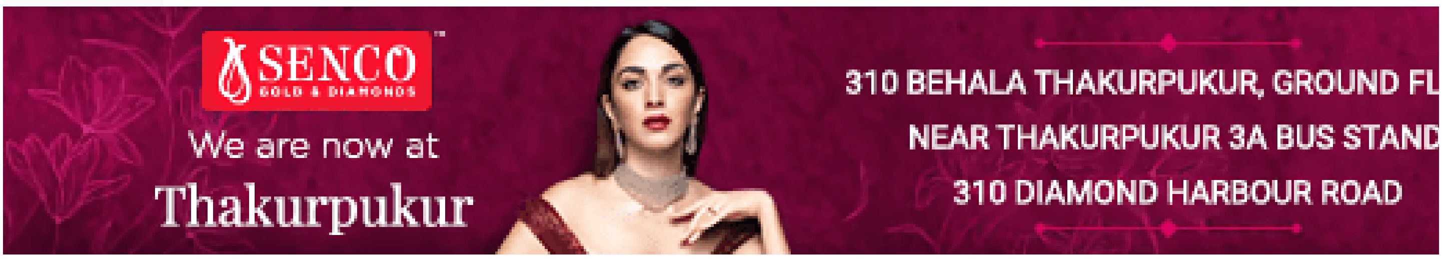
Torch AD ?

rentiation (AD) is a
culate the derivative of
function $f(x_1, \cdots, x_n)$ at some point.



AD is not symbolic math approach to calculate the derivate. Symbolic math approach would be to use derivation rules. For example, if you have $f(x) = \frac{1}{x}$ then $f'(x) = -\frac{1}{x^2}$.

AD is also not numeric procedure to calculate the derivate. The numerical procedure to calculate the derivative of `tanh` function at point $x = 1$ would be:

```
def tanh(x):
  y=np.exp(-x)
  return (1.0-y)/(1.0+y)

s=0.00001 # some small number
x=1.0
d=(tanh(x+s)-tanh(x))/s
print(d)
```

Output:

```
0.39322295790622513
```

How reverse mode AD works?

PyTorch uses **reverse mode** AD. AD *forward mode* exists, but it is computationally more expensive.

Reverse mode AD works the following way.

calculates the intermediate variables based on inputs.

The computational graph being calculated is like a tree. Inputs are *tree leaves* and each node in the graph corresponds to some operation (such as `+`), or to some function (such as `sin`).

The output function is *the root* of the tree. Once we create the computational tree in the forward pass, together with the intermediate gradients, we then may get the gradients from the root to any of the leaves.

We say: we compute the gradients of a function with respect to the input variable x.

This pass when we compute the gradients is known as the backward pass and corresponds to PyTorch [grad]() funciton.

PyTorch `grad` function is very cheap. It just traverses the computational graph and creates the sum of the intermediate gradient products to calculate the final gradient. The math behind calculating gradient is called the **chain rule**.

> NOTE:
> Note: There is one tool similar to Pytorch called Chainer just because of this chain rule principle.

Example:

To get a clue how PyTorch AD works the next code example we will create the computational graph for the function:

$$f(x_1, x_2) = \frac{1 + sin(x_2)}{x_2 + e^{x_1}} + x_1 x_2$$

We will calculate the gradient of a function $f(x_1, x_2)$ with respect to x_2.

```
import math
class ADNumber:
```

```
def __truediv__(self,other):
    new = ADNumber(self._val / other._
    self._children.append((1.0/other._
    other._children.append((-self._va
    return new

def __mul__(self,other):
    new = ADNumber(self._val*other._v
    self._children.append((other._val
    other._children.append((self._val
    return new

def __add__(self,other):
    if isinstance(other, (int, float)
        other = ADNumber(other, str(o
    new = ADNumber(self._val+other._v
    self._children.append((1.0,new))
    other._children.append((1.0,new))
    return new

def __sub__(self,other):
    new = ADNumber(self._val-other._v
    self._children.append((1.0,new))
    other._children.append((-1.0,new)
    return new


@staticmethod
def exp(self):
    new = ADNumber(math.exp(self._val
    self._children.append((self._val,
    return new

@staticmethod
def sin(self):
    new = ADNumber(math.sin(self._val
    self._children.append((math.cos(s
    return new
```

```
        else:
            result=0.0
            for child in other._children:
                result+=child[0]*self.gra
            return result

A = ADNumber # shortcuts
sin = A.sin
exp = A.exp

def print_child(f, wrt): # with respect t
    for e in f._children:
        print("child:", wrt, "->" , e[1].
        print_child(e[1], e[1].name)


x1 = A(1.5, name="x1")
x2 = A(0.5, name="x2")
f=(sin(x2)+1)/(x2+exp(x1))+x1*x2

print_childs(x2,"x2")
print("\ncalculated gradient for the func
```

Out:

```
child: x2 -> sin(x2) grad:  0.87758256189
child: sin(x2) -> sin(x2)+1 grad:  1.0
child: sin(x2)+1 -> sin(x2)+1/x2+exp(x1) 
child: sin(x2)+1/x2+exp(x1) -> sin(x2)+1/
child: x2 -> x2+exp(x1) grad:  1.0
child: x2+exp(x1) -> sin(x2)+1/x2+exp(x1)
child: sin(x2)+1/x2+exp(x1) -> sin(x2)+1/
child: x2 -> x1*x2 grad:  1.5
child: x1*x2 -> sin(x2)+1/x2+exp(x1)+x1*x

calculated gradient for the function f wi
```

Out:

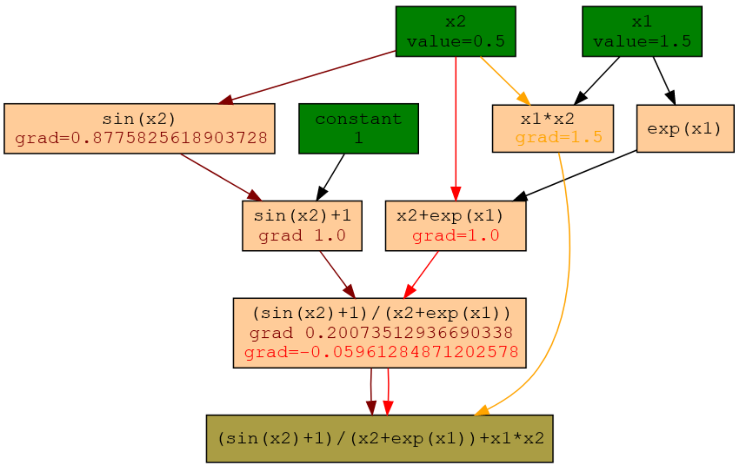
```
1.6165488003791768
```

The next image shows the computational graph for the example function:

$$f(x_1, x_2) = \frac{1 + sin(x_2)}{x_2 + e^{x_1}} + x_1 x_2$$

where

$$x_1 = 1.5, x_2 = 0.5$$



Each node in the tree graph is either a leaf node (green) or the root node (brown) or something in between.

From the input x2 in forward pass we identify three paths leading to the root. The arrows in dark red, red and orange denote these paths. We can ignore black

To compute the final gradient for our function `f` with respect to the `x2` we need to multiply the gradient values along the paths and finally to sum them up.

The calculus is as follows:

```
1.5 + (0.8775825618903728 * 1.0 * 0.20073
# 1.6165488003791768
```

This is exactly what our function `grad` will do if we print `f.grad(x2)` the result will be 1.6165488003791766.

Let's show the numerical procedure will provide the same result.

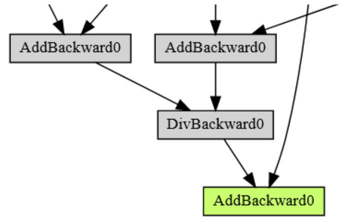
```
import math
def f(x1, x2):
    return (math.sin(x2)+1)/(x2+math.exp(

e=0.0001 # some small e
x1 = 1.5
x2 = 0.5

grad = (f(x1, x2+e)-f(x1, x2))/e
```

Create backward computational graph using torchviz

```
# !pip install torchviz
from torchviz import make_dot

# Create tensors
x1 = torch.tensor(1.5, requires_grad=True
x2 = torch.tensor(0.5, requires_grad=True
c = torch.tensor(1., requires_grad=True)

# Build a computational graph
y=(torch.sin(x2)+c)/(x2+torch.exp(x1))+x1
y.backward() # compute gradients

print(x1.grad)
print(x2.grad)
print(c.grad)

params = {'x1': x1, 'x2':x2, 'c': c}
param_map = {id(v): k for k, v in params.
param_map

make_dot(y, {'x1': x1, 'x2':x2, 'c': c})
```

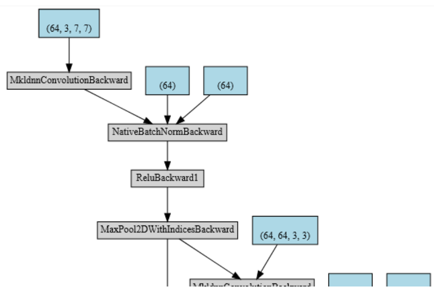
Out:

```
tensor(0.2328)
tensor(1.6165)
tensor(0.2007)
```



Example: Create resnet18 computational graph

```
import torch
import torchvision.models as models
resnet18 = models.resnet18()
x = torch.zeros(1, 3, 224, 224, dtype=tor
out = resnet18(x)
make_dot(out)
```



Example: Using hiddenlayer

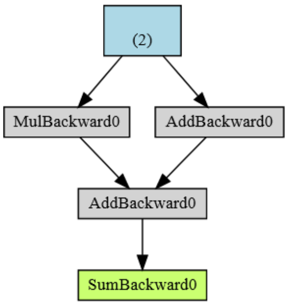
```
import torch
import hiddenlayer as hl
import torchvision.models as models
resnet18 = models.resnet18()
x = torch.zeros(1, 3, 224, 224, dtype=tor

transforms = [ hl.transforms.Prune('Const
# resnet18 from torchvision and and x is
graph = hl.build_graph(resnet18, x, trans
graph.theme = hl.graph.THEMES['blue'].cop
# graph.save('rnn_hiddenlayer', format='p
```

Save and zoom to check the details

Detach from AD

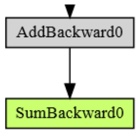
Here is one computational graph.

```
from torchviz import make_dot
x=torch.ones(2, requires_grad=True)
y=2*x
z=3+x
r=(y+z).sum()
make_dot(r)
```



It is possible to `detach()` the tensor from the AD computational graph.

```
from torchviz import make_dot
x=torch.ones(2, requires_grad=True)
y=2*x
z=3+x.detach()
r=(y+z).sum()
make_dot(r)
```



> NOTE:
> `x.detach()` is the same as `x.data`.

```
from torchviz import make_dot
x=torch.ones(2, requires_grad=True)
y=2*x
z=3+x.data
r=(y+z).sum()
make_dot(r)
```

You can use the `with torch.no_grad()` class (context manager). Whatever is created inside that block, will end as `requires_grad=False`. The next example will show just that. Tensor `x` that `requires_grad=True` will create tensor `y`, but that tensor will have `requires_grad=False`.

```
x=torch.tensor(2., requires_grad=True)
print(x)
with torch.no_grad():
    y = x * 2
print(y, y.requires_grad)
```

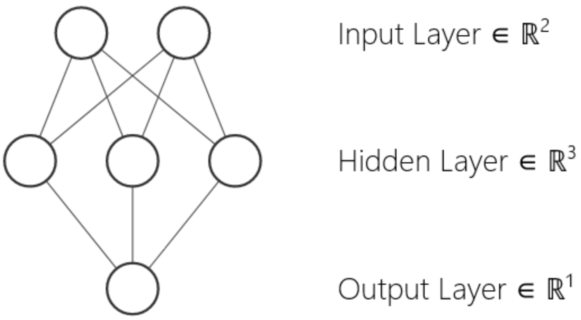
Out:

```
tensor(2., requires_grad=True)
tensor(4.) False
```

Bonus define deep learning

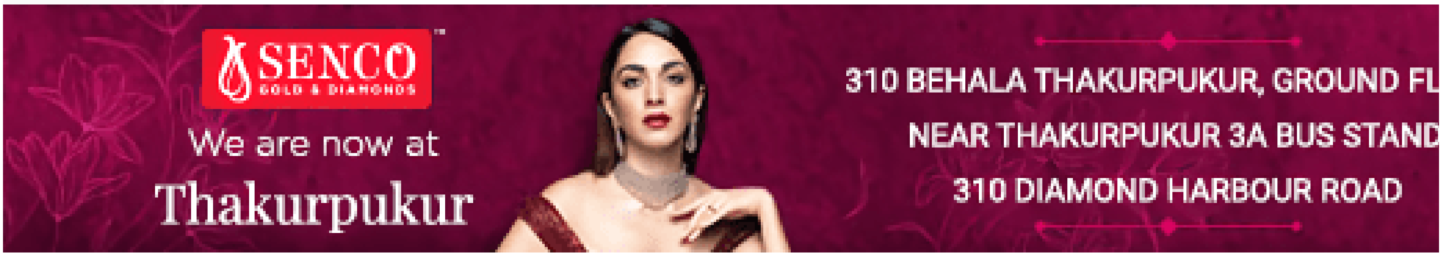
In essence, for the deep learning you need to have deep models. By definition, shallow models have just one hidden layer:

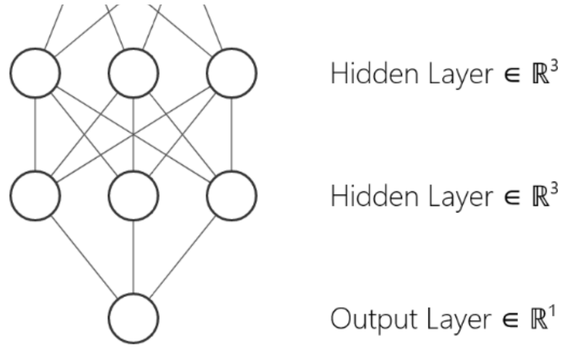
```
model = torch.nn.Sequential(
          torch.nn.Linear(D_in, H),
          torch.nn.Linear(H, D_out),
        )
```



Deep models have 2 or more hidden layers.

```
model = torch.nn.Sequential(
          torch.nn.Linear(D_in, H1),
          torch.nn.Linear(H1, H2),
          torch.nn.Linear(H2, D_out),
        )
```





In other words, to do some deep learning you need to have at least three linear layers. The dimension `H` is called the hidden dimension. Instead of `nn.Linear` layers you may use convolution layers.

...

tags: *ad - pytorch automatic differentiation - pytorch ad - automatic differentiation - computational graph - backward computational graph - reverse mode ad - derivation rule* & **category:** *pytorch*