GENERAL

- Look at Proposal Feedback
- PSET 4 Due Next Tuesday
- Recitation will be this Friday (Lopata 103, 10:30-Noon)

AUTOGRAD

Building Our Own Deep Learning Framework

- Computation Graph that encodes symbolic relationship between input to output (and loss)
- Nodes in this graph are:
  - Values: Values are set from training data
  - Params: Values are initialized and updated using SGD
  - Operations: Values are computed as functions of their input
- Forward computation to compute loss
- Backward computation to compute gradients for every node

AUTOGRAD

Code from pset5/mnist.py

```python
# Inputs and parameters
inp = edf.Value()
lab = edf.Value()

W1 = edf.Param()
B1 = edf.Param()
W2 = edf.Param()
B2 = edf.Param()

# Model
y = edf.matmul(inp,W1)
y = edf.add(y,B1)
y = edf.RELU(y)
y = edf.matmul(y,W2)
y = edf.add(y,B2) # This is our final prediction
```
BRIEF DETOUR

- What are RELUs?

Element-wise non-linear activations

\[ \text{RELU}(x) = \max(0, x) \]

- Previous activations would be sigmoid-like: \( \sigma(x) = \frac{\exp(x)}{1 + \exp(x)} \)
  - Great when you want a probability, bad when you want to learn by gradient descent.
  - For both high and low-values of \( x \), \( \frac{\text{d}\sigma(x)}{\text{d}x} = 0 \)
  - So if you weren’t careful, you would end up with high-magnitude activations, and the network stops learning.

Gradient descent is very fragile!

BRIEF DETOUR

- What are RELUs?

\[ \text{RELU}(x) = \max(0, x) \]

What is \( \text{d}\text{RELU}(x) / \text{d}x \)?

0 if \( x < 0 \), 1 otherwise.

- So your gradients are passed un-changed if the input is positive.
- But completely attenuated if the input is negative.
- So there’s still the possibility of your optimization getting stuck, if you reach a point where all inputs to the RELU are negative.
- Will talk about initialization, etc. later.

AUTOGRAD

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```

When you construct an object, it just does book-keeping!
AUTOGRAD

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```
At this point, we've just defined the graph: no actual computation has happened!

Now let's train this thing!

Beginning of training:

```
nHidden = 1024; K = 10
W1.set(xavier((28*28,nHidden)))
B1.set(np.zeros((nHidden)))
W2.set(xavier((nHidden,K)))
B2.set(np.zeros((K)))
```

Initialize weights randomly.

In each iteration of training:

```
for iters in range(...):
    ... inp.set(train_im[idx[b:b+BSZ],:]):
    ... lab.set(train_lb[idx[b:b+BSZ]])
    ...```

Load data into the 'values' or inputs.

What is this set function anyway?

```
class Value:
    def __init__(self):
        values.append(self)
    def set(self,value):
        self.top = np.float32(value).copy()

class Param:
    def __init__(self):
        params.append(self)
    def set(self,value):
        self.top = np.float32(value).copy()
```

Sets a member called "top" to be an array that holds these values.
Note that we are loading our input data in batches as matrices.
inp is BSZ x N
Then we're doing a matmul with W1 which is N x nHidden.
Output will be BSZ x nHidden
Essentially, we're replacing vector matrix multiply for a single sample with matrix-matrix multiply for a batch of samples.

And this will work. It will print the loss and accuracy values for the set inputs, given the current value of the parameters.
What is this magical function forward?

From edf.py

```
# Global forward
def Forward():
    for c in ops: c.forward()
```

But the operation classes have their own forward function.
```
class matmul:
    def __init__(self,x,y):
        ops.append(self)
        self.x = x
        self.y = y
    def forward(self):
        self.top = np.matmul(self.x.top,self.y.top)
    ...
```
So the forward pass computes the loss. But we want to learn the parameters.

The SGD function is pretty simple

```python
for iters in range(...):
    ...  
    inp.set(train_im[idx[b:b+BSZ,:,:])
    lab.set(train_lb[idx[b:b+BSZ]])
    edf.Forward()
    print(loss.top,acc.top)
    edf.Backward(loss)
    edf.SGD(lr)
```

The SGD function is pretty simple

```python
def SGD(lr):
    for p in params:
        p.top = p.top - lr*p.grad
```

This requires `p.grad` (gradients with respect to loss) to be present.

That's what **backward** does!

---

From edf.py

```python
# Global backward
def Backward(loss):
    for c in ops:
        c.grad = np.zeros_like(c.top)
    for c in params:
        c.grad = np.zeros_like(c.top)
    loss.grad = np.ones_like(loss.top)
    for c in ops[::-1]: c.backward()
```

- Called with an op object as the loss.
- Initializes all gradients to zero.
- `x.grad` is defined as the gradient of the loss wrt to `x.top`
- And so, initializes `loss.grad` to all ones.
- Each op has a backward function. Calls this in reverse order.
The backward function adds to the gradients of its inputs. Those inputs could've been used by other ops.
Computes gradients of its inputs based on the value of its own gradients (i.e., of its output).
Assumes that by the time backward is called on it, self.grad will exist and be final. Why?

Assumes that by the time backward is called on it, self.grad will exist and be final.
Because anything that could add to its gradient would have been called before it.
Only computes grads for params and ops (not values).
AUTOGRAD

- Allows us to specify a complex estimation function as a composition of simpler functions.
- Need to just provide an 'implementation' for each function so that we know how to:
  - Compute outputs given inputs
  - Compute contribution to gradients of inputs given gradient of output
- Given this model, can allow us to compute gradients of all parameters automatically!

SPATIAL OPERATIONS

Instead, consider our input to be what it is, an image!

- Work with 4-D arrays of size $B \times H \times W \times C$ instead of matrices.
- Use convolutional layers, which produce multi-channel output images from multi-channel input images, except that each output pixel only depends on a small number of input pixels in its neighborhood.
  - And this dependence is translation invariant.

$$g[b, y, x, c_2] = \sum_{k_y} \sum_{k_x} \sum_{c_1} f[b, y + k_y, x + k_x, c_1] k[k_y, k_x, c_1, c_2]$$

(Note that this is actually 'correlation' not convolution)

In the problem set, you'll have to implement forward and backward.

SPATIAL OPERATIONS

- So far, even though our inputs were images, we were treating them as vectors.
- inp is a matrix of size $B \times N$, where $B$ is the batch-size, and $N$ was the number of pixels ($28^2$ for MNIST).
- So each sample is represented by a row vector of size $N$.
- This means that parameters of the first layer $W_1 = N \times H$, where $H$ is the dimensionality of the encoding.
- That's a lot of weights, especially as you go to "real" images.
- We can't solve this by reducing $H$. Because then we would be assuming that there is a "linear" function that can reduce dimensionality and keep information required for classification.
- Need to do this slowly.

```python
y = edf.matmul(inp, W1)
for i in range(...):
    inp.set(train_im[idx[b:b+BSZ],:])
    lab.set(train_lb[idx[b:b+BSZ]])
    ...
```

```python
y = edf.conv2(inp, K1)
y = edf.down2(y); y = edf.down2(y);
y = edf.add(y, B1)
y = edf.RELU(y)
y = edf.flatten(y)
y = edf.matmul(y, W2)
y = edf.add(y, B2) # This is our final prediction
```
This is actually a huge waste of computation! We're computing values and then throwing them away.

```python
# Downsample by 2
class down2:
    def __init__(self, x):
        ops.append(self)
        self.x = x

    def forward(self):
        self.top = self.x.top[:,::2,::2,:]

    def backward(self):
        if self.x in ops or self.x in params:
            grd = np.zeros_like(self.x.top)
            grd[:,::2,::2,:] = self.grad
            self.x.grad = self.x.grad + grd
```

```python
y = edf.conv2(inp, K1)
y = edf.down2(y); y = edf.down2(y);
y = edf.add(y, B1)
y = edf.RELU(y)
y = edf.flatten(y)
y = edf.matmul(y, W2)
y = edf.add(y, B2)  # This is our final prediction
```

This is actually a huge waste of computation! We're computing values and then throwing them away.

```python
# Flatten (conv to fc)
class flatten:
    def __init__(self, x):
        ops.append(self)
        self.x = x

    def forward(self):
        self.top = np.reshape(self.x.top, [self.x.top.shape[0], -1])

    def backward(self):
        if self.x in ops or self.x in params:
            self.x.grad = self.x.grad + np.reshape(self.grad, self.x.top.shape)
```

**OTHER OPERATIONS**

View 1

- Neural network is a collection of neurons that mimic the brain

View 2

- Neural networks are programs with differentiable operations acting on inputs and trainable parameters.

- Variety of "basic" operations possible: as long as they're (at least partially) differentiable
- Express more complex operations in terms of these basic operations
- Design your network by writing a program
  - That you think can express the required computation to solve a problem (would work if you just have the right parameters).
  - Has a healthy gradient flow so that it can learn those parameters.
Conditional Operations

Consider `edf.max` which implements $z = \max(x, y)$

- Its forward function is very simple:
  
  ```python
  self.top = np.maximum(self.x.top, self.y.top)
  ```

- What about backward?

  \[
  \nabla_x \nabla z = \begin{cases} 
  1 & \text{if } x \geq y, \\
  0 & \text{otherwise}
  \end{cases}
  \]

  \[
  \nabla_y \nabla z = \begin{cases} 
  1 & \text{if } y \geq x, \\
  0 & \text{otherwise}
  \end{cases}
  \]

  - So we back-propagate to the input we picked.
  - But don’t back-propagate the "condition"

- `edf.where` selects from two inputs based on relative value of two other inputs.

  \[
  z = (p \geq q) x + (q > p) y
  \]

  - No gradients generated for the condition

    \[
    \nabla_p \nabla z = \begin{cases} 
    1 & \text{if } p \geq q, \\
    0 & \text{otherwise}
    \end{cases}
    \]

    \[
    \nabla_q \nabla z = \begin{cases} 
    1 & \text{if } q > p, \\
    0 & \text{otherwise}
    \end{cases}
    \]

    \[
    \nabla_z = 0
    \]

    - Can still be useful

      - But if you hope to learn parts of the network generating $p$ and $q$, they must have gradients coming from elsewhere.

EAGER EXECUTION

- Conditionals are tricky
  - You are often executing both execution paths of the condition and picking one.
  - Can get really hairy when the condition is to setup a loop (recurrent networks)

- Essentially, your computation graph must contain all possible execution paths, with the condition "masking" which values end up in your final solution.

- This can be inefficient.

- What if you added only the ops that are required based on the condition?

  But we don’t know the values of the conditions when we construct the graph!

Solution: Eager Execution (PyTorch, now in Tensorflow)

- Construct a separate graph for each iteration of training
- Params are initialized before training. Inputs are called with their values in each iteration.
- Object constructor for each operation node also calls forward
- You can therefore check the value of `top` as you are constructing the graph to decide which nodes to add.
- Once you have the final output, just call backward
  - Will compute gradients for all parameters (and operations) used in that iteration.
- Afterwards, delete the graph and start anew for the next iteration.