Homework 7: Computation Graphs, Back-propagation, and Neural Networks

Due: Friday, May 6th, 2022 at 11:59PM EST

Instructions: Your answers to the questions below, including plots and mathematical work, should be submitted as a single PDF file. It's preferred that you write your answers using software that typesets mathematics (e.g.LaTeX, LyX, or MathJax via iPython), though if you need to you may scan handwritten work. You may find the minted package convenient for including source code in your LaTeX document. If you are using LyX, then the listings package tends to work better.

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1 Introduction

There is no doubt that neural networks are a very important class of machine learning models. Given the sheer number of people who are achieving impressive results with neural networks, one might think that it's relatively easy to get them working. This is a partly an illusion. One reason so many people have success is that, thanks to GitHub, they can copy the exact settings that others have used to achieve success. In fact, in most cases they can start with "pre-trained" models that already work for a similar problem, and "fine-tune" them for their own purposes. It's far easier to tweak and improve a working system than to get one working from scratch. If you create a new model, you're kind of on your own to figure out how to get it working: there's not much theory to guide you and the rules of thumb do not always work. Understanding even the most basic questions, such as the preferred variant of SGD to use for optimization, is still a very active area of research.

One thing is clear, however: If you do need to start from scratch, or debug a neural network model that doesn't seem to be learning, it can be immensely helpful to understand the low-level details of how your neural network works – specifically, back-propagation. With this assignment, you'll have the opportunity to linger on these low-level implementation details. Every major neural network type (RNNs, CNNs, Resnets, etc.) can be implemented using the basic framework we'll develop in this assignment.

To help things along, Philipp Meerkamp, Pierre Garapon, and David Rosenberg have designed a minimalist framework for computation graphs and put together some support code. The intent is for you to read, or at least skim, every line of code provided, so that you'll know you understand all the crucial components and could, in theory, create your own from scratch. In fact, creating your own computation graph framework from scratch is highly encouraged – you'll learn a lot.

2 Computation Graph Framework

To get started, please read the tutorial on the computation graph framework we'll be working with. (Note that it renders better if you view it locally.) The use of computation graphs is not specific to machine learning or neural networks. Computation graphs are just a way to represent a function that facilitates efficient computation of the function's values and its gradients with respect to inputs. The tutorial takes this perspective, and there is very little in it about machine learning, per se.

To see how the framework can be used for machine learning tasks, we've provided a full implementation of linear regression. You should start by working your way through the `__init__` of the `LinearRegression` class in `linear_regression.py`. From there, you'll want to review the node class definitions in `nodes.py`, and finally the class `ComputationGraphFunction` in `graph.py`. `ComputationGraphFunction` is where we repackage a raw computation graph into something that's more friendly to work with for machine learning. The rest of `linear_regression.py` is fairly routine, but it illustrates how to interact with the `ComputationGraphFunction`.

As we've noted earlier in the course, getting gradient calculations correct can be difficult. To help things along, we've provided two functions that can be used to test the backward method of a node and the overall gradient calculation of a `ComputationGraphFunction`. The functions are in `test_utils.py`, and it's recommended that you review the tests provided for the linear regression implementation in `linear_regression.t.py`. (You can run these tests from the command line with `python3 linear_regression.t.py.`) The functions actually doing the testing, `test_node_backward` and `test_ComputationGraphFunction`, may seem a bit intricate, but they're implementing the exact same `gradient_checker` logic we saw in the second homework assignment.

Once you've understood how linear regression works in our framework, you're ready to start implementing your own algorithms. To help you get started, please make sure you are able to execute the following commands:

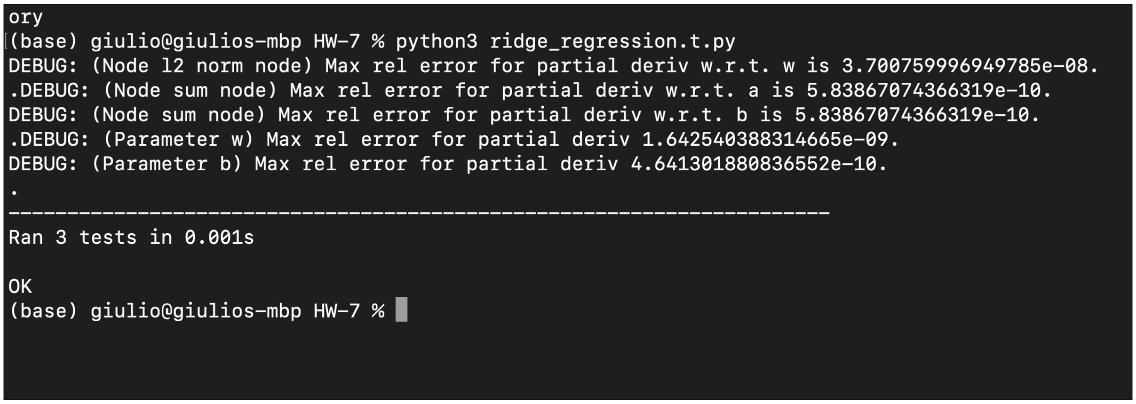
- cd /path/to/hw7
- python3 linear_regression.py
- python3 linear_regression.t.py

3 Ridge Regression

When moving to a new system, it's always good to start with something familiar. But that's not the only reason we're doing ridge regression in this homework. In ridge regression the parameter vector is "shared", in the sense that it's used twice in the objective function. In the computation graph, this can be seen in the fact that the node for the parameter vector has two outgoing edges. This sharing is common many popular neural networks (RNNs and CNNs), where it is often referred to as *parameter tying*.

`ridge_regression.py` provides a skeleton code and `ridge_regression.t.py` is a test code, which you should eventually be able to pass.

1. Complete the class `L2NormPenaltyNode` in `nodes.py`. If your code is correct, you should be able to pass test_L2NormPenaltyNode in `ridge_regression.t.py`. Please attach a screenshot that shows the test results for this question.



```
ory
(base) giulio@giulios-mbp HW-7 % python3 ridge_regression.t.py
DEBUG: (Node l2 norm node) Max rel error for partial deriv w.r.t. w is 3.700759996949785e-08.
.DEBUG: (Node sum node) Max rel error for partial deriv w.r.t. a is 5.83867074366319e-10.
DEBUG: (Node sum node) Max rel error for partial deriv w.r.t. b is 5.83867074366319e-10.
.DEBUG: (Parameter w) Max rel error for partial deriv 1.642540388314665e-09.
DEBUG: (Parameter b) Max rel error for partial deriv 4.641301880836552e-10.
.
----------------------------------------------------------------------
Ran 3 tests in 0.001s

OK
(base) giulio@giulios-mbp HW-7 %
```

Figure 1: Ridge Regression Test Output

```python
class L2NormPenaltyNode(object):
    """ Node computing l2_reg * ||w||^2 for scalars l2_reg and vector w"""
    def __init__(self, l2_reg, w, node_name):
        """
        Parameters:
        l2_reg: a numpy scalar array (e.g. np.array(.01)) (not a node)
        w: a node for which w.out is a numpy vector
        node_name: node's name (a string)
        """
        self.node_name = node_name
        self.out = None
        self.d_out = None
        self.l2_reg = np.array(l2_reg)
        self.w = w

    def forward(self):
        self.out = self.l2_reg * np.dot(self.w.out,self.w.out)
        self.d_out = np.zeros(self.out.shape)
        return self.out

    def backward(self):
        d_w = 2 * self.w.out * self.l2_reg * self.d_out
        self.w.d_out += d_w
        return self.d_out

    def get_predecessors(self):
```

```
        ## Your code
        return [self.w]
```

2. Complete the class `SumNode` in `nodes.py`. If your code is correct, you should be able to pass test_SumNode in `ridge_regression.t.py`. Please attach a screenshot that shows the test results for this question.

```
class SumNode(object):
    """ Node computing a + b, for numpy arrays a and b"""
    def __init__(self, a, b, node_name):
        """
        Parameters:
        a: node for which a.out is a numpy array
        b: node for which b.out is a numpy array of the same shape as a
        node_name: node's name (a string)
        """
        self.node_name = node_name
        self.out = None
        self.d_out = None
        self.b = b
        self.a = a

    def forward(self):
        self.out = self.a.out + self.b.out
        self.d_out = np.zeros(self.out.shape)
        return self.out

    def backward(self):
        #Derivative of a+b with respect to either is just 1
        self.a.d_out += self.d_out
        self.b.d_out += self.d_out
        return self.d_out

    def get_predecessors(self):
        # Your code
        return [self.a,self.b]
```

3. Implement ridge regression with w regularized and b unregularized. Do this by completing the `__init__` method in `ridge_regression.py`, using the classes created above. When complete, you should be able to pass the tests in `ridge_regression.t.py`. Report the average square error on the **training** set for the parameter settings given in the `main()` function.

```python
class RidgeRegression(BaseEstimator, RegressorMixin):
    """ Ridge regression with computation graph """
    def __init__(self, l2_reg=1, step_size=.005,  max_num_epochs = 5000):
        self.max_num_epochs = max_num_epochs
        self.step_size = step_size

        # Build computation graph
        self.x = nodes.ValueNode(node_name="x") # to hold a vector input
        self.y = nodes.ValueNode(node_name="y") # to hold a scalar response
        self.w = nodes.ValueNode(node_name="w") # to hold the parameter vector
        self.b = nodes.ValueNode(node_name="b") # to hold the bias parameter (scalar)
        self.prediction = nodes.VectorScalarAffineNode(x=self.x, w=self.w, b=self.b,
                                                        node_name="prediction")

        self.objective = nodes.SquaredL2DistanceNode(a=self.prediction, b=self.y,
                                                      node_name="square loss")
        self.reg_loss = nodes.L2NormPenaltyNode(l2_reg=l2_reg, w=self.w,node_name = "reg_loss'
        self.loss = nodes.SumNode(a = self.objective,b = self.reg_loss, node_name="loss")

        self.inputs = [self.x]
        self.outcomes = [self.y]
        self.parameters = [self.w, self.b]

        self.graph = graph.ComputationGraphFunction(self.inputs, self.outcomes,
                                                    self.parameters, self.prediction,
                                                    self.loss)
```

Epoch 0 : Ave objective= 1.6239215396574016 Ave training loss: 0.829453172961588
Epoch 50 : Ave objective= 0.3279290433014191 Ave training loss: 0.24172708726984105
Epoch 100 : Ave objective= 0.3162914498004661 Ave training loss: 0.21217722541565676
Epoch 150 : Ave objective= 0.31393109789649476 Ave training loss: 0.2035621043730588
Epoch 200 : Ave objective= 0.3125125713798402 Ave training loss: 0.2001356855415311
Epoch 250 : Ave objective= 0.3119400564708615 Ave training loss: 0.19965745539619076
Epoch 300 : Ave objective= 0.31207381347038765 Ave training loss: 0.19790617941810598
Epoch 350 : Ave objective= 0.31071724617823365 Ave training loss: 0.19849725926934042
Epoch 400 : Ave objective= 0.30909123840416197 Ave training loss: 0.19769513064580496
Epoch 450 : Ave objective= 0.3095956300923911 Ave training loss: 0.19947123786346668
Epoch 500 : Ave objective= 0.3106691495858917 Ave training loss: 0.19746671340931904
Epoch 550 : Ave objective= 0.3097702703398206 Ave training loss: 0.1975530030565645
Epoch 600 : Ave objective= 0.3096404461483278 Ave training loss: 0.19757342715060294
Epoch 650 : Ave objective= 0.3083718030493469 Ave training loss: 0.19798154668862517
Epoch 700 : Ave objective= 0.3061819997787804 Ave training loss: 0.20096498299523102
Epoch 750 : Ave objective= 0.30749345254109606 Ave training loss: 0.20011306539220786
Epoch 800 : Ave objective= 0.308886136728931 Ave training loss: 0.19780391185875232
Epoch 850 : Ave objective= 0.3087756131500073 Ave training loss: 0.1979265611692196
Epoch 900 : Ave objective= 0.3079008111420143 Ave training loss: 0.19828758687030695
Epoch 950 : Ave objective= 0.30714000150784715 Ave training loss: 0.19918632705454822
Epoch 1000 : Ave objective= 0.3066139625516689 Ave training loss: 0.1983538577667799
Epoch 1050 : Ave objective= 0.30747453428905724 Ave training loss: 0.19820704824051763

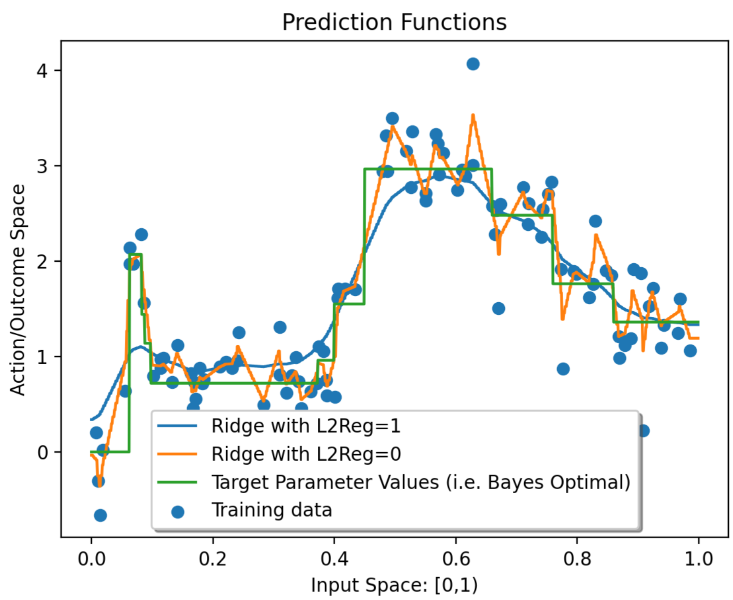
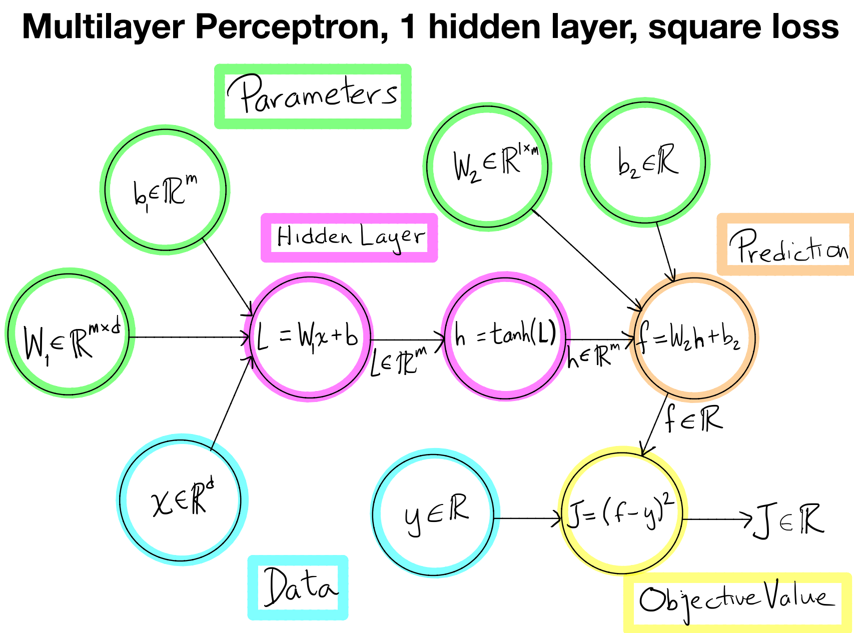


Figure 2: Plot of Ridge Regression Function

Epoch 1100 : Ave objective= 0.307717086685998 Ave training loss: 0.19846361621089495
Epoch 1150 : Ave objective= 0.3071694530616267 Ave training loss: 0.19842395292093531
Epoch 1200 : Ave objective= 0.30674000718540045 Ave training loss: 0.19898645299672726
Epoch 1250 : Ave objective= 0.30699547023638646 Ave training loss: 0.19895396194344603
Epoch 1300 : Ave objective= 0.30642748711226797 Ave training loss: 0.1985901886833973
Epoch 1350 : Ave objective= 0.30615191656287044 Ave training loss: 0.199005159544057
Epoch 1400 : Ave objective= 0.3060371837844445 Ave training loss: 0.19891405876500912
Epoch 1450 : Ave objective= 0.3062969093476848 Ave training loss: 0.19899046363269882
Epoch 1500 : Ave objective= 0.305438561622688 Ave training loss: 0.19894348007805548
Epoch 1550 : Ave objective= 0.30504945078923296 Ave training loss: 0.19973854031118024
Epoch 1600 : Ave objective= 0.3056182509567906 Ave training loss: 0.1993384607112306
Epoch 1650 : Ave objective= 0.30516021965519713 Ave training loss: 0.1997367416480982
Epoch 1700 : Ave objective= 0.30612457725427844 Ave training loss: 0.1994450493029651
Epoch 1750 : Ave objective= 0.30534247389005786 Ave training loss: 0.19963722970707437
Epoch 1800 : Ave objective= 0.30323881967916166 Ave training loss: 0.19947349139237075
Epoch 1850 : Ave objective= 0.30511616661964014 Ave training loss: 0.19967194537598545
Epoch 1900 : Ave objective= 0.3051455341157816 Ave training loss: 0.19947225697730386

4 Multilayer Perceptron

Let's now turn to a multilayer perceptron (MLP) with a single hidden layer and a square loss. We'll implement the computation graph illustrated below:



The crucial new piece here is the nonlinear **hidden layer**, which is what makes the multilayer perceptron a significantly larger hypothesis space than linear prediction functions.

4.1 The standard non-linear layer

The multilayer perceptron consists of a sequence of "layers" implementing the following non-linear function

$$h(x) = \sigma(Wx + b),$$

where $x \in \mathbb{R}^d$, $W \in \mathbb{R}^{m \times d}$, and $b \in \mathbb{R}^m$, and where m is often referred to as the number of **hidden units** or **hidden nodes**. σ is some non-linear function, typically tanh or ReLU, applied element-wise to the argument of σ. Referring to the computation graph illustration above, we will implement this nonlinear layer with two nodes, one implementing the affine transform $L = W_1 x + b_1$, and the other implementing the nonlinear function $h = \tanh(L)$. In this problem, we'll work out how to implement the backward method for each of these nodes.

The Affine Transformation

In a general neural network, there may be quite a lot of computation between any given affine transformation $Wx + b$ and the final objective function value J. We will capture all of that in a function $f : \mathbb{R}^m \to \mathbb{R}$, for which $J = f(Wx + b)$. Our goal is to find the partial derivative of J with respect to each element of W, namely $\partial J / \partial W_{ij}$, as well as the partials $\partial J / \partial b_i$, for each element of b. For convenience, let $y = Wx + b$, so we can write $J = f(y)$. Suppose we have already computed the partial derivatives of J with respect to the entries of $y = (y_1, \ldots, y_m)^T$, namely $\frac{\partial J}{\partial y_i}$ for $i = 1, \ldots, m$. Then by the chain rule, we have

$$\frac{\partial J}{\partial W_{ij}} = \sum_{r=1}^{m} \frac{\partial J}{\partial y_r} \frac{\partial y_r}{\partial W_{ij}}.$$

4. Show that $\frac{\partial J}{\partial W_{ij}} = \frac{\partial J}{\partial y_i} x_j$, where $x = (x_1, \ldots, x_d)^T$. [Hint: Although not necessary, you might find it helpful to use the notation $\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & \text{else} \end{cases}$. So, for examples, $\partial_{x_j} \left(\sum_{i=1}^n x_i^2 \right) = 2x_i \delta_{ij} = 2x_j$.]

   To answer this question we must calculate $\frac{\partial y_r}{\partial W_{ij}}$:
   If we nudge the entry i, j of the weight matrix W we have changes corresponding as following:

$$\frac{\partial y_r}{\partial W_{ij}} \rightarrow \begin{cases} x_j & if\ r = j \\ 0 & if\ otherwise \end{cases}$$

   This is clear to see by the definition of matrix - vector multiplication. If we have Ax = b then $b_i = \langle A_i, x \rangle$ where A_i is the i^{th} row of the matrix A. If we hold all of the other indices of the W matrix constant, that is to say $W_{r,k}$ is constant where $r, j \neq i, j$, then when we take the partial derivative of y with respect to $W_{i,j}$, those constants go to 0. Therefore, when we evaluate the derivative of our dot product $\langle A_i, x \rangle$, we get a summation of 0's with one term that is non zero, x_j:

$$\frac{\partial y_r}{\partial W_{ij}} \rightarrow \langle W_i, x \rangle = \sum_{r=1}^{d} \delta_{ij} \times x_r = x_j \ where\ \delta_{ij} \rightarrow \begin{cases} x_j & if\ r = j \\ 0 & if\ otherwise \end{cases}$$

   Therefore, what we have is:

$$\frac{\partial J}{\partial W_{ij}} = \frac{\partial J}{\partial y_i} x_j$$

5. Now let's vectorize this. Let's write $\frac{\partial J}{\partial y} \in \mathbb{R}^{m \times 1}$ for the column vector whose ith entry is $\frac{\partial J}{\partial y_i}$. Let's also define the matrix $\frac{\partial J}{\partial W} \in \mathbb{R}^{m \times d}$, whose ij'th entry is $\frac{\partial J}{\partial W_{ij}}$. Generally speaking, we'll always take $\frac{\partial J}{\partial A}$ to be an array of the same size ("shape" in numpy) as A. Give a vectorized expression for $\frac{\partial J}{\partial W}$ in terms of the column vectors $\frac{\partial J}{\partial y}$ and x. [Hint: Outer product.]

   We want a matrix $\frac{\partial J}{\partial W} \in \mathbb{R}^{m \times d}$ whose ij'th takes the form $\frac{\partial J}{\partial W_{ij}}$. If we're given $\frac{\partial J}{\partial y} \in \mathbb{R}^{m \times 1}$ then what we need is a vector in $\mathbb{R}^{1 \times d}$ to take the outer product with to create our $\frac{\partial J}{\partial W}$ matrix.
   We know from the last problem that

$$\frac{\partial J}{\partial W_{ij}} = \frac{\partial J}{\partial y_i} x_j$$

   Its easy to see that if we take the outer product of the vector $\frac{\partial J}{\partial y} \in \mathbb{R}^{m \times 1}$and the vector $x \in \mathbb{R}^{1 \times d}$ then we'll have a matrix

$$\frac{\partial J}{\partial y} \otimes x = \frac{\partial J}{\partial y} x^T \rightarrow \left(\frac{\partial J}{\partial y} \otimes x \right)_{i,j} = \left(\frac{\partial J}{\partial y} \right)_i x_j \ therefore\ \frac{\partial J}{\partial y} \otimes x = \frac{\partial J}{\partial W}$$

6. In the usual way, define $\frac{\partial J}{\partial x} \in \mathbb{R}^d$, whose i'th entry is $\frac{\partial J}{\partial x_i}$. Show that

$$\frac{\partial J}{\partial x} = W^T \left(\frac{\partial J}{\partial y} \right)$$

[Note, if x is just data, technically we won't need this derivative. However, in a multilayer perceptron, x may actually be the output of a previous hidden layer, in which case we will need to propagate the derivative through x as well.]

Using the chain rule, we know that Then the partial of J with respect to an x_j is:

$$\frac{\partial J}{\partial x_j} = \sum_{i=1}^{m} \frac{\partial J}{\partial y_i} \frac{\partial y_i}{\partial x_j}$$

If we consider the change of x_j as it corresponds to the output of y_i:

$$\frac{\partial y_i}{\partial x_j} = W_{ij}$$

Therefore, if were summing over m, we have:

$$\frac{\partial J}{\partial x_j} = \sum_{i=1}^{m} \frac{\partial J}{\partial y_i} W_{ij} = \langle \frac{\partial J}{\partial y}, W_j \rangle = \langle W_j, \frac{\partial J}{\partial y}, \rangle = W_j^T \frac{\partial J}{\partial y}$$

Where we can see that the partial derivative of J with respect to x_j is a linear combination of the entries of W scaled by the partial derivatives of J with respect to y_i. If we compute all of the partial derivatives at once, we arrive at our desired equivalency:

$$\frac{\partial J}{\partial x} = W^T \frac{\partial J}{\partial y}$$

7. Show that $\frac{\partial J}{\partial b} = \frac{\partial J}{\partial y}$, where $\frac{\partial J}{\partial b}$ is defined in the usual way.

The vector b, is just the linear bias term, a vector with values are equal to a single variable. Hence, its derivative will always be 1:

$$\frac{\partial y_i}{\partial b} = 1$$

Using the chain rule:

$$\frac{\partial J}{\partial b} = \frac{\partial J}{\partial y_i} \frac{y_i}{b} = \sum_{i=1}^{m} \frac{\partial J}{\partial y_i} \times 1 = \frac{\partial J}{\partial y}$$

Element-wise Transformers

Our nonlinear activation function nodes take an array (e.g. a vector, matrix, higher-order tensor, etc), and apply the same nonlinear transformation $\sigma : \mathbb{R} \to \mathbb{R}$ to every element of the array.

Let's abuse notation a bit, as is usually done in this context, and write $\sigma(A)$ for the array that results from applying $\sigma(\cdot)$ to each element of A. If σ is differentiable at $x \in \mathbb{R}$, then we'll write $\sigma'(x)$ for the derivative of σ at x, with $\sigma'(A)$ defined analogously to $\sigma(A)$.

Suppose the objective function value J is written as $J = f(\sigma(A))$, for some function $f : S \mapsto \mathbb{R}$, where S is an array of the same dimensions as $\sigma(A)$ and A. As before, we want to find the array $\frac{\partial J}{\partial A}$ for any A. Suppose for some A we have already computed the array $\frac{\partial J}{\partial S} = \frac{\partial f(S)}{\partial S}$ for $S = \sigma(A)$. At this point, we'll want to use the chain rule to figure out $\frac{\partial J}{\partial A}$. However, because we're dealing with arrays of arbitrary shapes, it can be tricky to write down the chain rule. Appropriately, we'll use a tricky convention: We'll assume all entries of an array A are indexed by a single variable. So, for example, to sum over all entries of an array A, we'll just write $\sum_i A_i$.

8. Show that $\frac{\partial J}{\partial A} = \frac{\partial J}{\partial S} \odot \sigma'(A)$, where we're using $\odot$ to represent the **Hadamard product**. If A and B are arrays of the same shape, then their Hadamard product $A \odot B$ is an array with the same shape as A and B, and for which $(A \odot B)_i = A_i B_i$. That is, it's just the array formed by multiplying corresponding elements of A and B. Conveniently, in `numpy` if `A` and `B` are arrays of the same shape, then `A*B` is their Hadamard product.

We know that the derivative of the non linear transformation $\sigma(\cdot)$ is $\sigma'(\cdot)$, therefore, applying the derivative to A we have $\frac{\partial \sigma}{\partial A} = \sigma'(A)$. We want to compute $\frac{\partial J}{\partial A}$, using the chain rule we know this is equal to:

$$\frac{\partial J}{\partial A} = \frac{\partial J}{\partial S} \frac{\partial S}{\partial A}$$

Lets observe what happens when we change a single entry, i, from our array A.

$$\frac{\partial S}{\partial A_i} = \frac{\partial \sigma(A)}{\partial A_i} = \sigma'(A_i)$$

Where $S = \sigma(A)$ and $f(S)$ maps S to $\mathbb{R}$ for every element of the array. Since what we have is a an arbitrary mapping of every element of S through $f(S)$, and the mapping of $\mathbb{R}$ to $\mathbb{R}$ from $\sigma'(A)$ each element of S is a multiplication of two reals, dependent on the inputs of A_i and the output of $\sigma(A_i)$:

$$\frac{\partial J}{\partial A_i} = \frac{\partial J}{\partial S_i} \frac{\partial S}{\partial A_i} = \frac{\partial J}{\partial S_i} \frac{\partial \sigma(A)}{\partial A_i} = \frac{\partial J}{\partial S_i} \sigma'(A) \rightarrow \frac{\partial J}{\partial A} = \frac{\partial J}{\partial S} \odot \sigma'(A)$$

where $\odot$ is the element wise Hadamard product.

4.2 MLP Implementation

```
Epoch  450 : Ave objective= 0.05148649345246612  Ave training loss:  0.04602761810834408
(base) giulio@giulios-mbp HW-7 % python3 mlp_regression.t.py
DEBUG: (Node affine) Max rel error for partial deriv w.r.t. W is 1.73108695787578e-08.
DEBUG: (Node affine) Max rel error for partial deriv w.r.t. b is 2.8043132239587723e-09.
DEBUG: (Node affine) Max rel error for partial deriv w.r.t. x is 1.6690539911771478e-07.
.DEBUG: (Node tanh) Max rel error for partial deriv w.r.t. a is 1.94415814934202e-08.
.DEBUG: (Parameter W1) Max rel error for partial deriv 1.505724385157152e-07.
DEBUG: (Parameter b1) Max rel error for partial deriv 2.430644738943934e-08.
DEBUG: (Parameter w2) Max rel error for partial deriv 2.2883519281334212e-08.
DEBUG: (Parameter b2) Max rel error for partial deriv 6.892198988201343e-10.
.
----------------------------------------------------------------------
Ran 3 tests in 0.003s

OK
```

Figure 3: MLP Test Outputs

9. Complete the class `AffineNode` in `nodes.py`. Be sure to propagate the gradient with respect to x as well, since when we stack these layers, x will itself be the output of another node that depends on our optimization parameters. If your code is correct, you should be able to pass test_AffineNode in `mlp_regression.t.py`. Please attach a screenshot that shows the test results for this question.

```python
class AffineNode(object):
    """Node implementing affine transformation (W,x,b)-->Wx+b, where W is a matrix,
    and x and b are vectors
        Parameters:
        W: node for which W.out is a numpy array of shape (m,d)
        x: node for which x.out is a numpy array of shape (d)
        b: node for which b.out is a numpy array of shape (m) (i.e. vector of length m)
    """
    def __init__(self, W, x, b,node_name):
        """
        Parameters:
        W: node for which w.out is a numpy matrix
        x: node for which a.out is a numpy array
        b: node for which b.out is a numpy array of the same shape as a
        node_name: node's name (a string)
        """
        self.node_name = node_name
        self.out = None
        self.d_out = None
        self.W = W
        self.b = b
        self.x = x

    def forward(self):
        self.out = np.matmul(self.W.out, self.x.out) + self.b.out
```

```
        self.d_out = np.zeros(self.out.shape)
        return self.out

    def backward(self):
        #Use derivatives we calculated in homework
        self.W.d_out = np.ma.outer(self.d_out, self.x.out)
        self.b.d_out = self.d_out
        self.x.d_out = np.matmul(self.W.out.T, self.d_out)
        return self.d_out

    def get_predecessors(self):
        # Your code
        return [self.W,self.b,self.x]
```

10. Complete the class `TanhNode` in `nodes.py`. As you'll recall, $\frac{d}{dx}\tanh(x) = 1 - \tanh^2 x$. Note that in the forward pass, we'll already have computed tanh of the input and stored it in self.out. So make sure to use `self.out` and not recalculate it in the backward pass. If your code is correct, you should be able to pass test_TanhNode in `mlp_regression.t.py`. Please attach a screenshot that shows the test results for this question.

```
class TanhNode(object):
    """Node tanh(a), where tanh is applied elementwise to the array a
        Parameters:
        a: node for which a.out is a numpy array
    """
    def __init__(self, a,node_name):
        """
        Parameters:
        a: node for which a.out is a numpy array
        node_name: node's name (a string)
        """
        self.node_name = node_name
        self.out = None
        self.d_out = None
        self.a = a

    def forward(self):
        self.out = np.tanh(self.a.out)
        self.d_out = np.zeros(self.out.shape)
        return self.out

    def backward(self):
        #Use derivatives we calculated in homework
        self.a.d_out = self.d_out * (1 - (self.out**2))
        return self.d_out

    def get_predecessors(self):
        return [self.a]
```

11. Implement an MLP by completing the skeleton code in `mlp_regression.py` and making use of the nodes above. Your code should pass the tests provided in `mlp_regression.t.py`. Note that to break the symmetry of the problem, we initialize our weights to small random values, rather than all zeros, as we often do for convex optimization problems. Run the MLP for the two settings given in the `main()` function and report the average **training** error. Note that with an MLP, we can take the original scalar as input, in the hopes that it will learn nonlinear features on its own, using the hidden layers. In practice, it is quite challenging to get such a neural network to fit as well as one where we provide features.

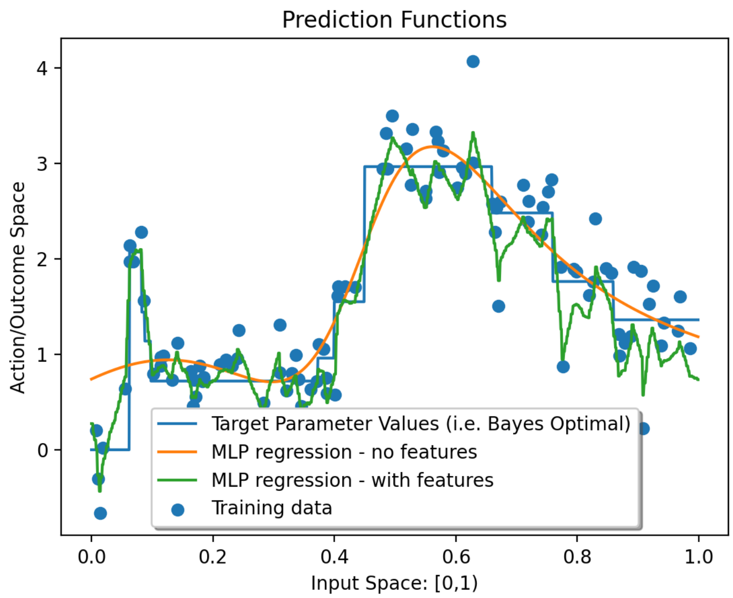


Figure 4: MLP Plot output

```
class MLPRegression(BaseEstimator, RegressorMixin):
    """ MLP regression with computation graph """
    def __init__(self, num_hidden_units=10, step_size=.005, init_param_scale=0.01, max_num_epo
        #Given Params
        self.num_hidden_units = num_hidden_units
        self.init_param_scale = init_param_scale
        self.max_num_epochs = max_num_epochs
        self.step_size = step_size
        #Value Nodes
        self.y = nodes.ValueNode(node_name="y")  # to hold a vector input
        self.x = nodes.ValueNode(node_name="x")  # to hold a vector input
        self.W1 = nodes.ValueNode(node_name="W1")
        self.w2 = nodes.ValueNode(node_name="w2")
        self.b1 = nodes.ValueNode(node_name="b1")
        self.b2 = nodes.ValueNode(node_name="b2")
```

```
        #Package Arguments
        self.inputs = [self.x]
        self.outcomes = [self.y]
        self.parameters = [self.W1, self.b1, self.w2, self.b2]
        #Transformation Nodes
        self.matrixAffineNode = nodes.AffineNode(
            W=self.W1, x=self.x, b=self.b1, node_name="Matrix-Vector Affine Node")
        self.tanh = nodes.TanhNode(
            a=self.matrixAffineNode, node_name="TanH node")
        self.prediction = nodes.VectorScalarAffineNode(
            x=self.tanh, b=self.b2, w=self.w2, node_name="Vector
    Scalar Affine Prediction Node")
        self.objective = nodes.SquaredL2DistanceNode(
            a=self.prediction, b=self.y, node_name="Squared Distance Node")
        self.graph = graph.ComputationGraphFunction(self.inputs, self.outcomes,
                                                    self.parameters, self.prediction,
                                                    self.objective)
```

Epoch 0 : Ave objective= 3.1384886539883388 Ave training loss: 2.723785243910098
Epoch 50 : Ave objective= 0.9452874177705872 Ave training loss: 0.943461455298143
Epoch 100 : Ave objective= 0.9445033731029092 Ave training loss: 0.942652506502907
Epoch 150 : Ave objective= 0.9367476670890391 Ave training loss: 0.9346090461873809
Epoch 200 : Ave objective= 0.8844483557361549 Ave training loss: 0.8810580089341782
Epoch 250 : Ave objective= 0.7915298648457691 Ave training loss: 0.7875920118136019
Epoch 300 : Ave objective= 0.7675597340207823 Ave training loss: 0.7633388588307334
Epoch 350 : Ave objective= 0.7602930361825055 Ave training loss: 0.7564261106066077
Epoch 400 : Ave objective= 0.7524547326529253 Ave training loss: 0.7484077188972953
Epoch 450 : Ave objective= 0.7428788443128451 Ave training loss: 0.738966672345131
Epoch 500 : Ave objective= 0.7321920184466244 Ave training loss: 0.7288235006540531
Epoch 550 : Ave objective= 0.7222214365888472 Ave training loss: 0.7187396934421737
Epoch 600 : Ave objective= 0.7130055930160536 Ave training loss: 0.7092100547107983
Epoch 650 : Ave objective= 0.7044883875478416 Ave training loss: 0.7007717624558434
Epoch 700 : Ave objective= 0.6969450741027985 Ave training loss: 0.6935702346255589
Epoch 750 : Ave objective= 0.6910156523283387 Ave training loss: 0.6875683109990217
Epoch 800 : Ave objective= 0.6862222329256947 Ave training loss: 0.6824991754483698
Epoch 850 : Ave objective= 0.6819994828642706 Ave training loss: 0.6781000976663271
Epoch 900 : Ave objective= 0.6773895074147217 Ave training loss: 0.6740627739647225
Epoch 950 : Ave objective= 0.6736227015552761 Ave training loss: 0.669864085725015
Epoch 1000 : Ave objective= 0.6693218243530432 Ave training loss: 0.6653432766719775
Epoch 1050 : Ave objective= 0.6643837895234525 Ave training loss: 0.6601950629134805
Epoch 1100 : Ave objective= 0.6585088963124851 Ave training loss: 0.6539338279490771
Epoch 1150 : Ave objective= 0.6510972305836367 Ave training loss: 0.6462104106767659
Epoch 1200 : Ave objective= 0.6415259617630464 Ave training loss: 0.6364378999285787
Epoch 1250 : Ave objective= 0.6295993066336498 Ave training loss: 0.6242604999266641
Epoch 1300 : Ave objective= 0.6142219153217402 Ave training loss: 0.6082239068761517
Epoch 1350 : Ave objective= 0.5954813684673169 Ave training loss: 0.5888388672455861
Epoch 1400 : Ave objective= 0.5709948524358075 Ave training loss: 0.5659841940822471
Epoch 1450 : Ave objective= 0.5430969069160582 Ave training loss: 0.5404888850053465
Epoch 1500 : Ave objective= 0.5146237289009121 Ave training loss: 0.5082343319474094

Epoch 1550 : Ave objective= 0.48356823492449197 Ave training loss: 0.47586773954280814
Epoch 1600 : Ave objective= 0.4514673318252107 Ave training loss: 0.44358943167442194
Epoch 1650 : Ave objective= 0.42216074491521666 Ave training loss: 0.4138969070261208
Epoch 1700 : Ave objective= 0.3959897535492102 Ave training loss: 0.3882628148595082
Epoch 1750 : Ave objective= 0.37463870229920154 Ave training loss: 0.36757513611321946
Epoch 1800 : Ave objective= 0.3594697433958645 Ave training loss: 0.3520927159473004
Epoch 1850 : Ave objective= 0.34629722997211343 Ave training loss: 0.34081126371663695
Epoch 1900 : Ave objective= 0.33292407430679505 Ave training loss: 0.334826289682421
Epoch 1950 : Ave objective= 0.33221653382092337 Ave training loss: 0.3246279741340167
Epoch 2000 : Ave objective= 0.3254469869100473 Ave training loss: 0.3195559080130552
Epoch 2050 : Ave objective= 0.3191475404122815 Ave training loss: 0.31602858351100305
Epoch 2100 : Ave objective= 0.3194399126729073 Ave training loss: 0.310987799563054
Epoch 2150 : Ave objective= 0.31347039708863256 Ave training loss: 0.3095644700210537
Epoch 2200 : Ave objective= 0.30925097045693034 Ave training loss: 0.30628300955673343
Epoch 2250 : Ave objective= 0.30815239160309493 Ave training loss: 0.302177619523987
Epoch 2300 : Ave objective= 0.305460336189331 Ave training loss: 0.29903566851895924
Epoch 2350 : Ave objective= 0.3026997974708049 Ave training loss: 0.29636267413752004
Epoch 2400 : Ave objective= 0.3004278784672875 Ave training loss: 0.29484270071893703
Epoch 2450 : Ave objective= 0.2986209840718123 Ave training loss: 0.29220179992469186
Epoch 2500 : Ave objective= 0.29228630014181634 Ave training loss: 0.29300318803571096
Epoch 2550 : Ave objective= 0.2950618790412984 Ave training loss: 0.28805881036612
Epoch 2600 : Ave objective= 0.2923601903618309 Ave training loss: 0.2866935017033392
Epoch 2650 : Ave objective= 0.29148179187751955 Ave training loss: 0.28448913111610524
Epoch 2700 : Ave objective= 0.28896976044790185 Ave training loss: 0.2829393560287766
Epoch 2750 : Ave objective= 0.2868191289049734 Ave training loss: 0.28137306934023487
Epoch 2800 : Ave objective= 0.28531300657157144 Ave training loss: 0.2798083898582309
Epoch 2850 : Ave objective= 0.2842080841525052 Ave training loss: 0.2781184660054683
Epoch 2900 : Ave objective= 0.28271008763298594 Ave training loss: 0.27661781946323705
Epoch 2950 : Ave objective= 0.2806229154132455 Ave training loss: 0.27540973147311154
Epoch 3000 : Ave objective= 0.2796565925441325 Ave training loss: 0.2738203206425151
Epoch 3050 : Ave objective= 0.2764865169964034 Ave training loss: 0.27447982849389996
Epoch 3100 : Ave objective= 0.2763603740746643 Ave training loss: 0.2715763865913923
Epoch 3150 : Ave objective= 0.27558867438514956 Ave training loss: 0.2703350929006941
Epoch 3200 : Ave objective= 0.27444147940519065 Ave training loss: 0.2686737759054997
Epoch 3250 : Ave objective= 0.27203739375033714 Ave training loss: 0.26824221780073015
Epoch 3300 : Ave objective= 0.27179551223861614 Ave training loss: 0.2663827986195835
Epoch 3350 : Ave objective= 0.26964341016686966 Ave training loss: 0.26626356176210825
Epoch 3400 : Ave objective= 0.26804093348640645 Ave training loss: 0.2655768577899346
Epoch 3450 : Ave objective= 0.26632823817318807 Ave training loss: 0.2642029002460602
Epoch 3500 : Ave objective= 0.2673348358188661 Ave training loss: 0.26265675013281986
Epoch 3550 : Ave objective= 0.2647839016616244 Ave training loss: 0.2622159813318914
Epoch 3600 : Ave objective= 0.26462533335380395 Ave training loss: 0.26204829869432755
Epoch 3650 : Ave objective= 0.2639994700194897 Ave training loss: 0.25906637418812495
Epoch 3700 : Ave objective= 0.2617166615490344 Ave training loss: 0.2596774688183659
Epoch 3750 : Ave objective= 0.26165028350887537 Ave training loss: 0.2574431609637332
Epoch 3800 : Ave objective= 0.26174575538285344 Ave training loss: 0.2563592205344483
Epoch 3850 : Ave objective= 0.26050615894939877 Ave training loss: 0.25603940761988975
Epoch 3900 : Ave objective= 0.25938168132136885 Ave training loss: 0.2546501240398735
Epoch 3950 : Ave objective= 0.2587562436576191 Ave training loss: 0.2542149655292055

Epoch 4000 : Ave objective= 0.2573923586445567 Ave training loss: 0.2534187670327716
Epoch 4050 : Ave objective= 0.2575037498261381 Ave training loss: 0.25222824572726765
Epoch 4100 : Ave objective= 0.2567433957573593 Ave training loss: 0.2514705797058361
Epoch 4150 : Ave objective= 0.254539201860611 Ave training loss: 0.25081065052643925
Epoch 4200 : Ave objective= 0.2551022001931922 Ave training loss: 0.2500129556752864
Epoch 4250 : Ave objective= 0.2524591307616317 Ave training loss: 0.2511660755294462
Epoch 4300 : Ave objective= 0.253606426978595 Ave training loss: 0.2485668066428239
Epoch 4350 : Ave objective= 0.25224274642086864 Ave training loss: 0.24804124753794388
Epoch 4400 : Ave objective= 0.25171003798259906 Ave training loss: 0.24718285629754916
Epoch 4450 : Ave objective= 0.2518032563510767 Ave training loss: 0.24668291744528095
Epoch 4500 : Ave objective= 0.2509992469334581 Ave training loss: 0.24596185427796008
Epoch 4550 : Ave objective= 0.25049238776736305 Ave training loss: 0.2452602339866061
Epoch 4600 : Ave objective= 0.24667098437191168 Ave training loss: 0.24469438801640678
Epoch 4650 : Ave objective= 0.24868314822435666 Ave training loss: 0.24402846433041894
Epoch 4700 : Ave objective= 0.24835918306678365 Ave training loss: 0.24374840714503526
Epoch 4750 : Ave objective= 0.24813844789514078 Ave training loss: 0.24286703419961467
Epoch 4800 : Ave objective= 0.2467084452633521 Ave training loss: 0.2436449712832135
Epoch 4850 : Ave objective= 0.2460279568646779 Ave training loss: 0.24217766666977902
Epoch 4900 : Ave objective= 0.2465078880032288 Ave training loss: 0.24132104095532025
Epoch 4950 : Ave objective= 0.24568467743447064 Ave training loss: 0.24067333063364513
Epoch 0 : Ave objective= 3.2800713177228773 Ave training loss: 2.853580140086361
Epoch 50 : Ave objective= 0.14933163110436884 Ave training loss: 0.14641707217182806
Epoch 100 : Ave objective= 0.11796958226228409 Ave training loss: 0.10897419879235355
Epoch 150 : Ave objective= 0.10134139201573841 Ave training loss: 0.09053530456233325
Epoch 200 : Ave objective= 0.08369303494526008 Ave training loss: 0.08057937150782428
Epoch 250 : Ave objective= 0.07773935817925802 Ave training loss: 0.06512939388553708
Epoch 300 : Ave objective= 0.06421651532868872 Ave training loss: 0.10111298800424694
Epoch 350 : Ave objective= 0.06279796009585302 Ave training loss: 0.05203375968856143
Epoch 400 : Ave objective= 0.0527607128276177 Ave training loss: 0.04706368772606726
Epoch 450 : Ave objective= 0.049430156701997664 Ave training loss: 0.04412280461792682

4.3 Multiclass classification with an MLP (Optional)

We consider a generic classification problem with K classes over inputsn x of dimension d. Using a MLP we will compute a K-dimensional vector z representing scores,

$$z = W_2 \tanh(W_1 x + b_1) + b_2,$$

with $W_1 \in \mathbb{R}^{m\times d}$, $b_1 \in \mathbb{R}^m$, $W_2 \in \mathbb{R}^{K\times m}$ and $b_1 \in \mathbb{R}^K$. Our model assumes that x belongs to class k with probability

$$e^{z_k} / \sum_{k=1}^{K} e^{z_k},$$

which corresponds to applying a Softmax to the scores. Given this probabilistic model we can train the model by minimizing the negative log-likelihood.

12. Implement a Softmax node. We provided skeleton code for class SoftmaxNode in `nodes.py`. If your code is correct, you should be able to pass test_SoftmaxNode in `multiclass.t.py`. Please attach a screenshot that shows the test results for this question.

```
(base) giulio@giulios-mbp HW-7 % python3 multiclass.t.py
DEBUG: (Node softmax) Max rel error for partial deriv w.r.t. z is 4.7262207759012645e-08.
.DEBUG: (Parameter W1) Max rel error for partial deriv 1.4311740486199725e-06.
DEBUG: (Parameter b1) Max rel error for partial deriv 4.089499216263753e-09.
DEBUG: (Parameter W2) Max rel error for partial deriv 7.536304174674168e-09.
DEBUG: (Parameter b2) Max rel error for partial deriv 2.0273836877219766e-09.
.
----------------------------------------------------------------------
Ran 2 tests in 0.003s

OK
(base) giulio@giulios-mbp HW-7 %
```

Figure 5: Multiclass test

```python
class SoftmaxNode(object):
    """ Softmax node
        Parameters:
        z: node for which z.out is a numpy array
    """
    def __init__(self,z,node_name) -> None:
        self.node_name = node_name
        self.z = z
        self.d_out = None
        self.out = None

    def forward(self):
        self.out = np.exp(self.z.out) /  np.sum(np.exp(self.z.out))
        self.d_out = np.zeros(self.out.shape)
        return self.out

    def backward(self):
        jacobian = -np.outer(self.out, self.out)
        np.fill_diagonal(jacobian, self.out*(1-self.out))
        self.z.d_out = self.d_out @ jacobian
        return self.d_out

    def get_predecessors(self):
        return [self.z]
```

13. Implement a negative log-likelihood loss node for multiclass classification. We provided skeleton code for class NLLNode in `nodes.py`. The test code for this question is combined with the test code for the next question.

```python
class NLLNode(object):
    """ Node computing NLL loss between 2 arrays.
        Parameters:
        y_hat: a node that contains all predictions
        y_true: a node that contains all labels
```

```
    """
    def __init__(self,y_hat,y_true,node_name) -> None:
        self.out = None
        self.d_out = None
        self.y_hat = y_hat
        self.y_true = y_true
        self.node_name = node_name
        self.temp = None

    def forward(self):
        self.temp = self.y_hat.out[self.y_true.out]
        self.out = -np.log(self.temp)
        self.d_out = np.zeros(self.out.shape)
        return self.out

    def backward(self):
        self.temp2 = np.zeros(self.y_hat.out.shape)
        self.temp2[self.y_true.out] = -1*(self.temp**-1)
        self.y_hat.d_out = self.d_out * self.temp2
        return self.d_out

    def get_predecessors(self):
        return [self.y_hat,self.y_true]
```

14. Implement a MLP for multiclass classification by completing the skeleton code in `multiclass.py`. Your code should pass the tests in test_multiclass provided in multiclass.t.py. Please attach a screenshot that shows the test results for this question.

```
class MulticlassClassifier(BaseEstimator, RegressorMixin):
    """ Multiclass prediction """
    def __init__(self, num_hidden_units=10, step_size=.005, init_param_scale=0.01,
                                                    max_num_epochs=1000, num_class=3):
        self.num_hidden_units = num_hidden_units
        self.init_param_scale = init_param_scale
        self.max_num_epochs = max_num_epochs
        self.step_size = step_size
        self.num_class = num_class

        # Build computation graph
        # TODO: add your code here
        self.z = nodes.ValueNode(node_name='z')
        self.x = nodes.ValueNode(node_name='x')
        self.y = nodes.ValueNode(node_name='y')
        self.W1 = nodes.ValueNode(node_name='W1')
        self.W2 = nodes.ValueNode(node_name='W2')
        self.b1 = nodes.ValueNode(node_name='b1')
        self.b2 = nodes.ValueNode(node_name='b2')
```

```python
        # Package inputs / parameters into lists
        self.inputs = [self.x, self.z]
        self.outcomes = [self.y]
        self.parameters = [self.W1, self.b1, self.W2, self.b2]

        # First We Start With Affine Transformation W_1x+b_1
        self.MatVecAffine1 = nodes.AffineNode(
            W=self.W1, x=self.x, b=self.b1, node_name="Mat-Vec Affine Node 1")
        # Which feeds into a tahn layer
        self.tahnNode = nodes.TanhNode(
            a=self.MatVecAffine1, node_name="TahnNode")
        # Tahn node feeds into another Affine transformation -> W_2tahn + b_1
        self.MatVecAffine2 = nodes.AffineNode(
            W=self.W2, x=self.tahnNode, b=self.b2, node_name="Mat-Vec Affine Node 2")
        # Which becomes z, and fed into our softmax, creates prediction
        self.prediction = nodes.SoftmaxNode(
            z=self.MatVecAffine2, node_name="SoftMax Prediction Node")
        # Finally evaluated againts objective of NLL
        self.objective = nodes.NLLNode(
            y_hat=self.prediction, y_true=self.y, node_name="NLL Objective Node")

        # Build Computation Graph
        self.graph = graph.ComputationGraphFunction(
            inputs=self.inputs, outcomes=self.outcomes, parameters=self.parameters,
            prediction=self.prediction, objective=self.objective)
```

Epoch 0 Ave training loss: 0.10767753468425854 Epoch 50 Ave training loss: 0.003740272949801889
Epoch 100 Ave training loss: 0.0019509875089186053 Epoch 150 Ave training loss: 0.0013189220100329906
Epoch 200 Ave training loss: 0.0009947600104512845 Epoch 250 Ave training loss: 0.0007975221227264001
Epoch 300 Ave training loss: 0.0006649220947379011 Epoch 350 Ave training loss: 0.0005697138957458585
Epoch 400 Ave training loss: 0.0004980771960410213 Epoch 450 Ave training loss: 0.00044225221211177576
Epoch 500 Ave training loss: 0.0003975450315101266 Epoch 550 Ave training loss: 0.0003609495175393885
Epoch 600 Ave training loss: 0.0003304520224436157 Epoch 650 Ave training loss: 0.0003046529432352649
Epoch 700 Ave training loss: 0.0002825495526238341 Epoch 750 Ave training loss: 0.00026340479431621313
Epoch 800 Ave training loss: 0.00024666486030361454 Epoch 850 Ave training loss: 0.00023190568395950022
Epoch 900 Ave training loss: 0.0002187970217752761 Epoch 950 Ave training loss: 0.00020707801611844284
Test set accuracy = 1.000