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 \texttt{minted} package convenient for including source code in your \LaTeX document. If you are using \LyX, then the \texttt{listings} package tends to work better.

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. The reason so many people have success is that, thanks to GitHub, they can copy the exact settings that others have used to achieve success. 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 and suggestions 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 is implemented. With this assignment, you'll have an opportunity to linger on these low-level implementation details, which one usually rushes through in more specialized neural network classes. Every major neural network type (RNNs, CNNs, Resnets, etc) can be implemented using the basic building blocks we’ll develop in this assignment.

To help things along, we\textsuperscript{1} have designed a minimal 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 \texttt{tutorial} on the computation graph framework we’ll be working with. (Note that it renders better if you view it locally.) In some sense, computation graphs have nothing

\textsuperscript{1}Philipp Meerkamp, Pierre Garapon, and David Rosenberg
to do with machine learning or neural networks. They are just a way to represent a function that facilitates efficient computation of the function value and it's gradients with respect to inputs. The tutorial takes this perspective, and there is very little 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 test_ComputationGraphFunction are a bit intricate so they can work with any node or ComputationGraphFunction, but it’s using the exact same gradient_checker logic we saw in the first homework assignment.

Once you’ve understood how linear regression works in our framework, you’re ready to start implementing your own algorithms...

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. As we discussed in class, 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. While we don’t have this sharing in the multilayer perceptron, we do have it in RNNs and CNNs, the two neural network architectures that have had the most impact. So being able to handle ridge regression is a necessary condition (and possibly sufficient) for being able to represent the these important architectures.

We’ve provided some skeleton code in ridge_regression.py, and some test code in ridge_regression.t.py, that you should eventually be able to pass.

1. Complete the class L2NormPenaltyNode in nodes.py.
2. Complete the class SumNode in nodes.py.
3. Implement ridge regression with w regularized and b unregularized. Do this by completing the __init__ method in the 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.
4. [Optional] Create a new implementation of ridge regression that supports efficient minibatching. You will replace the the ValueNode x, which contains a vector, with a ValueNode
x, which contains a matrix. The convention is that the first dimension indexes examples and the second is features (as we have always done). Many of the nodes will have to be adapted to this use case. Demonstrate its use and speedup.

4 Multilayer Perceptron

In this problem, we’ll be implement a multilayer perceptron, with a single hidden layer, for the regression setting. 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. \( \sigma \) is some non-linear function, typically tanh or ReLU applied element-wise to the argument of \( \sigma \). Referring to the computation graph illustration above, we will implement this non-linear layer with two nodes, one implementing the affine transform \( L(x) = W_1x + b_1 \), and the other implementing the nonlinear function \( h(L) = \text{tanh}(L) \). In this problem we’ll work out how to implement the backward method for each of these nodes.
4.1.1 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 \( f : \mathbb{R}^m \rightarrow \mathbb{R} \), for which \( J = f(Wx + b) \). Our goal is to find the partial derivative of \( J \) with respect to each element of \( W \), namely \( \partial J / \partial W_{ij} \). 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 intermediate variable \( y = (y_1, \ldots, y_m)^T \), namely \( \frac{\partial J}{\partial y_i} \) for \( i = 1, \ldots, m \). Then by the chain rule, we have

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

1. 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, \( \partial x_i \left( \sum_{i=1}^n x_i^2 \right) = 2x_i \delta_{ij} = 2x_j \).]

2. Now let’s vectorize this. Let’s write \( \frac{\partial J}{\partial y} \in \mathbb{R}^{m \times 1} \) for the column vector whose \( i \)th 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.]

3. 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.]

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

4.1.2 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 \( \sigma : \mathbb{R} \rightarrow \mathbb{R} \) 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 \( \sigma \) is differentiable at \( x \in \mathbb{R} \), then we’ll write \( \sigma'(x) \) for the derivative of \( \sigma \) 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 \( f : S \rightarrow \mathbb{R} \), 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 \( \sum_i A_i \).
1. Show that $\frac{\partial J}{\partial A} = \frac{\partial J}{\partial S} \circ \sigma'(A)$, where we’re using $\circ$ to represent the Hadamard product. If $A$ and $B$ are arrays of the same shape, then their Hadamard product $A \circ B$ is an array with the same shape as $A$ and $B$, and for which $(A \circ B)_i = A_i B_i$. 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.

4.2 MLP Implementation

1. 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.

2. 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.

3. 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.

4. [Optional] See if you can get a fit on the training set with an MLP that uses just the scalar input that is about as good as the fit using the featurized inputs. You can do that by tweaking model parameters (e.g. the number of hidden nodes or layers) and/or the parameters of optimization. You may use any neural network framework (PyTorch, TensorFlow, etc), which can help by providing more advanced optimization techniques (e.g. Adam), variable initialization methods, and/or various normalization approaches (batch norm, etc).

4.3 [OPTIONAL]

1. [Optional] Implement a Softmax node.

2. [Optional] Implement a negative log-likelihood loss node for multiclass classification.

3. [Optional] Use the classes above to apply an MLP to the simple multiclass classification dataset we had on a previous assignment.