PROJECT 5
FEEDFORWARD NEURAL NETWORKS

DAVID ATLAS

Abstract. This paper will introduce feed-forward neural networks, a technique for learning non-linear functions. The backpropogation algorithm will be used in conjunction with gradient descent. Networks of 0, 1 and 2 hidden layers will be applied to several different real-world classification problems. The size of the hidden layer will be tuned using a validation set. A sigmoid activation function will be used to introduce non-linearities into the network. A softmax classifier will be used to train a multi-net classifier. The networks mostly outperform a naive baseline, although require substantial tuning effort to converge to a good solution.

1. Problem Statement & Hypothesis

Feed-forward neural networks are a popular technique for estimating non-linear relationships between a set of inputs, and the densities of a corresponding class label or regression target. In a feed-forward neural network, an affine transformation is conducted on an input, at which point a non-linear function (which will be called an activation function) is applied. This is the basic unit of a network. Many of these units can be combined, with the effect being a flexible model that can learn non-linearities and feature interactions.

Therefore, the hypothesis is that the networks should outperform naive baselines across all the real-world experiments run in this paper, as it is known from previous experiments that a simple linear classifier can outperform baseline on these problems. As such, the feed-forward network has *at least* as much capacity as those models, and should outperform.

However, the additional cost of the expanded model capacity is that the networks can be difficult to train. They are sensitive to the learning rate, number of iterations and size of each of the units. Therefore, it would not be wholly unexpected if it were to be too difficult to find a network that outperforms a simpler linear model on problems with classes that are largely linearly seperable.

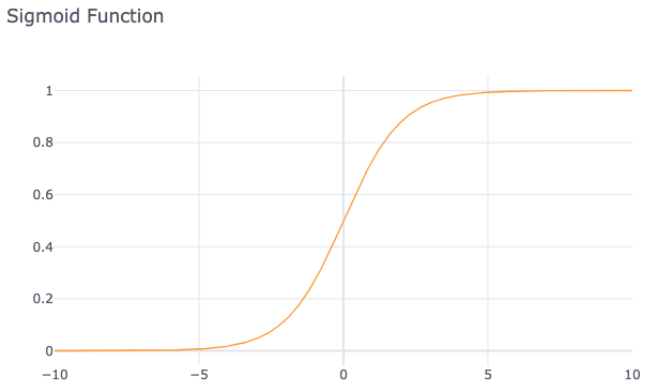
In the experiments below, 3 network configurations are used. A network with 0, 1 and 2 hidden layers will be applied to each problem. It is expected that the network with no hidden layers will perform in-line or better that the networks with hidden layers on problems with linear seperability. If an experiment presents a non-linear boundary between classes, it is expected that the hidden layer networks will outperform.

2. Description of Algorithms

Single Unit. The networks discussed in this paper are all composed of simple, small units. Each unit takes an input X and generates an output z via the following function:

$$\sigma(x) = \frac{1}{1 + \exp -x} z = \sigma(XW)$$

where W is a matrix with the same number of rows as X has columns. $sigma(x)$ is the sigmoid activation function, shown below in Figure 2. The sigmoid function plays two roles in the network. First, it introduces non-linearity. This is important, because several sequential linear transformations create a linear transformation, meaning that the network would only be able to create linear functions. Adding in the sigmoidal activation changes that. Second, the function maps from an unbounded space to the $[0, 1]$ interval. When training a classifier, the output must be interpreted as binary. The output of the sigmoid function can be interpreted as the probability of a positive predictions. This is also advantageos relative to a binary label because the interpretation is naturally probablistic.



Network Topology. Now that the basic unit of the network has been established, there are two parameters that must be chosen within the network.

The number of additional units to include in the network (which will be called the hidden layers) is crucial in defining the capacity of the network. As the number of units grows, the capacity of the network increases, all else equal, which reflects a change in the representation bias. However, the search space becomes bigger, and the selection bias plays a large role in whether the network converges to a performant solution.

Beyond the number of hidden layers, the size of each hidden layer must be chosen. Above, W was defined as a $m \times k$ (where X is $n \times m$). This leaves k as a parameter. In the experiments conducted here, k will be tuned over a validation set. Note that the effect of a larger value of k is similar to adding more units in the network - larger values will increase the representation capacity, but will create more parameters (and thus a larger search space).

There is also a relationship between the two parameters. A network might have fewer large hidden layers, or many small hidden layers. Fewer layers may be easier to train, but many layers can give more capacity with fewer parameters. Both should be chosen based on the problem.

Backpropogation. Given the network defined above, the challenge is in tuning the weight matrices W_h for each of the h units in the network. As in past papers, gradient descent will be used, but the challenge remains in calculating the gradient. Given the loss function

$$E(W, X) = (O - Y)^T (O - y)$$

, where $o_i \in O$ is the output of the network given input X_i, and Y is a vector of targets corresponding rowwise to X, the derivative of the loss relative to the output of the network is

$$\frac{dE}{dO} = (O - y).$$

At this point, the chain rule must be applied to find the derivative of the loss relative to the weights in the final layer. The derivative of the sigmoid function is

$$\sigma'(x) = \sigma(x)(1 - \sigma(x)),$$

and so

$$\frac{dE}{dW_H} = \frac{dE}{dO}\frac{\partial O}{\partial W_H} = (O - Y)\sigma(X)(1 - \sigma(X))X.$$

Next, the derivative for each of the preceding units must be found. First, δ_i is defined as

$$\delta_i = -\frac{\partial E}{\partial O_i},$$

where O_i is the output of the i^{th} layer. Using the chain rule, this can be written as

$$\begin{aligned}\delta_i &= -\frac{\partial E}{\partial O_{i+1}}\frac{\partial O_{i+1}}{\partial O_i} \\ &= \delta_{i+1}\frac{\partial O_{i+1}}{\partial O_i} \\ &= \delta_{i+1}W_{i+1}\frac{\partial O_i}{\partial X_i} \\ &= \delta_{i+1}W_{i+1}O_i(1-O_i).\end{aligned}$$

Practically, the delta rule will be leveraged. Rather than recalculating the derivative for each unit, the derivative can be expressed as the cumulative effect of all the units downstream from a given unit. This cumulative effect will be denoted δ_j for the j^{th} unit in the network:

$$\delta_j = \delta_{j+1}W_{j+1} \circ O_j(1-O_j),$$

where $A \circ B$ denotes the Hadamard (element-wise) product of A and B, and O_j indicates the output of the j^{th} unit. This is where the term *backpropogation* comes from - the derivative of the error is propogated backwards through each of the preceding units, all without having to recalculate the individual quantities, by accumulated δ_i throughout the network.

Gradient Descent. Having presented the delta-rule, calculating the gradient updates is easy.

$$\Delta W_h = \eta\delta_h X_h,$$

where η is the learning rate, δ_h is as defined above (the sum over all of the downstream δ_i), and X_h is the input to the h^{th} unit (the output of the $h-1^{th}$ unit or the original set of features if $h=1$)