THE INCREDIBLE SHRINKING NEURAL NETWORK: PRUNING TO OPERATE IN CONSTRAINED MEMORY ENVIRONMENTS

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ABSTRACT

We propose and evaluate a method for pruning neural networks to operate in constrained memory environments such as mobile or embedded devices. We evaluate a simple pruning technique using first-order derivative approximations of the gradient of each neuron in an optimally trained network, and turning off those neurons which contribute least to the output of the network. We then show the limitations of this type of approximation by comparing against the ground truth value for the change in error resulting from the removal of a given neuron. We attempt to improve on this using a second-order derivative approximation. We also explore the correlation between neurons in a trained network and attempt to improve our choice of candidate neurons for removal to account for faults that can occur from the removal of a single neuron at a time. We argue that this method of pruning allows for the optimal tradeoff in network size versus accuracy in order to operate within the memory constraints of a particular device or application environment.

1 INTRODUCTION

Neural network pruning algorithms were first popularized by Sietsma & Dow (1988) as a mechanism to determine the proper size network required to solve a particular problem. To this day, network design and optimal pruning remain inherently difficult tasks. For problems which cannot be solved using linear threshold units alone, Baum & Haussler (1989) demonstrate there is no way to precisely determine the appropriate size of a neural network a priori given any random set of training instances. Using too few neurons inhibits learning, and so in practice it is common to attempt to over-parameterize networks initially using a large number of hidden units and weights. However, as Chauvin (1990) writes, this approach can lead to over-fitting as the network's unnecessary free parameters start to latch on to idiosyncrasies in the training data.

Pruning algorithms, as comprehensively surveyed by Reed (1993), are a useful set of heruristics designed to identify and remove network parameters which do not contribute significantly to the output of the network and potentially inhibit generalization performance. At the time of Reed's writing, reducing network size was also a practical concern, as smaller networks are preferable in situations where computational resources are scarce. In this paper we are particularly concerned with application domains in which space is limited and network size constraints must be imposed with minimal impact on performance.

2 RELATED WORK

Neural network over-fitting is fundamentally a problem arising from the use of too many free parameters. Regardless of the number of weights used in a given network, as Segee & Carter (1991) assert, the representation of a learned function approximation is almost never evenly distributed over the hidden units, and the removal of any single hidden unit at random can actually result in a total network fault. Mozer & Smolensky (1989b) suggest that only a subset of the hidden units in a neural network actually latch on to the invariant or generalizing properties of the training inputs, and the rest learn to either mutually cancel each other out or begin over-fitting to the noise in the data. Determining which elements are unnecessary and removing them outright is therefore a well-founded approach to improving network generalization, and simultaneously provides a way to reduce their size in memory.

The generalization performance of neural networks has been well studied, and apart from pruning algorithms many heuristics have been used to avoid overfitting, such as dropout (Srivastava et al. (2014)), maxout (Goodfellow et al. (2013)), and cascade correlation (Fahlman & Lebiere (1989)), among others. However, these algorithms do not explicitly prioritize the reduction of network memory footprint as a part of their optimization criteria per se, (although in the opinion of the authors Fahlman's cascade correlation architecture holds great promise in this regard.) Computer memory size and processing capabilities have improved so much since the introduction of pruning algorithms in the late 1980s that space complexity has become a relatively negligible concern. The proliferation of cloud-based computing services has furthermore enabled mobile and embedded devices to leverage the power of massive data and computing centers remotely. In this domain, however, it is also reasonable to suggest that certain performance-critical applications running on low-resource devices could benefit from the ability to use neural networks locally.

At present there are few (if any) mechanisms specifically designed to shrink neural networks down in order to meet an externally imposed constraint on byte-size in memory. Without explicitly removing parameters from the network, one could use weight quantization to reduce the number of bytes used to represent each weight parameter, as investigated by Balzer et al. (1991), Dundar & Rose (1994), and Hoehfeld & Fahlman (1992). Of course, this method can only reduce the size of the network by a factor proportional to the byte-size reduction of each weight parameter.

Another method which has recently gained popularity is using the singular values of a trained weight matrix as basis vectors from which to derive a compressed hidden layer.

If we wanted to continually shrink a network to its absolute minimal size in an optimal manner, we might accomplish this using any number of off-the-shelf pruning algorithms, such as Skeletonization (Mozer & Smolensky (1989a)), Optimal Brain Damage (LeCun et al. (1989)), or later variants such as Optimal Brain Surgeon (Hassibi & Stork (1993)). In fact, we borrow much of our inspiration from these antecedent algorithms, with one major variation.

The aforementioned strategies all focus on the targeting and removal of *weight* parameters. Scoring and ranking individual weight parameters in a large network computationally expensive, and generally speaking the removal of a single weight from a large network is a drop in the bucket in terms of reducing a network's core memory footprint. We therefore train our sights on the ranking and removal of entire neurons along with their associated weight parameters. We argue that this is more efficient computationally as well as practically in terms of quickly reaching a target reduction in memory size. Our approach also attacks the angle of giving downstream applications a realistic expectation of the minimal increase in error resulting from the removal of a specified percentage of neurons from a trained network. Such trade-offs are unavoidable, but performance impacts can be limited if a principled approach is used to find candidate neurons for removal.

3 Experimental Results & Conclusions

Both versions of the proposed algorithm were run on 4 pattern recognition datasets, starting from a cosine wave and increasing in complexity to a distributed random shape pattern. These patterns are shown in Figure **??**. In all cases, the models were trained on a 2-hidden layer network with 50 neurons in each layer. Median thresholding produced much better results in all the cases and hence is used for all the results presented here.

The results of pruning using ground truth, first-order Taylor Series approximation and second-order Taylor Series approximation for both the variations of the proposed algorithm are shown in Figures, **??**, 3, 4 and 5.

It can be seen in all the cases that first-order Taylor Series expansion based pruning is a very bad approximation of the ground truth while ranking based on second-order expansion approximates the ground truth with much more accuracy. Also, it can be observed that the Iterative Re-Ranking

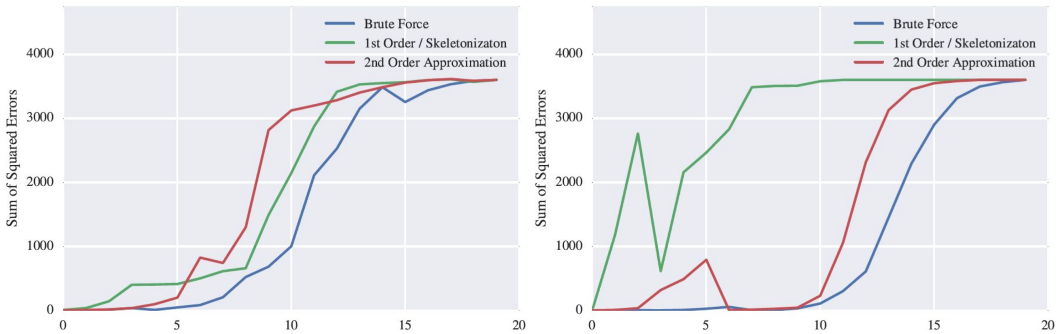

Figure 1: (Starting training accuracy: 0.9999993) Performance degradation using a small network with two layers of ten neurons each. Vertical axes represent the sum of squared errors on the training set, and horizontal axes represent the number of neurons removed. The left graph represents the single-pass overall ranking procedure (Algorithm 1) and the right represents continual re-estimation procedure (Algorithm 2).

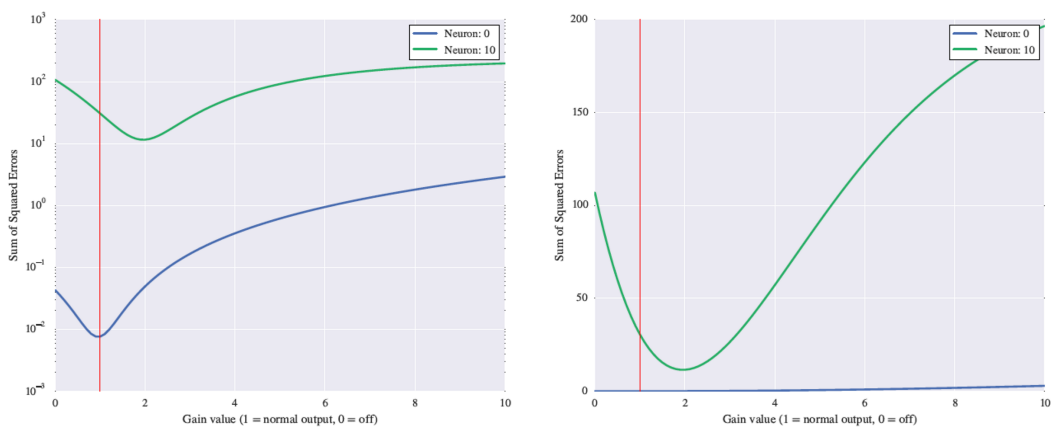

Figure 2: (Starting training accuracy: 0.9999993) Performance degradation using a small network with two layers of ten neurons each. Vertical axes represent the sum of squared errors on the training set, and horizontal axes represent the number of neurons removed. The left graph represents the single-pass overall ranking procedure (Algorithm 1) and the right represents continual re-estimation procedure (Algorithm 2).

version of the algorithm always performs better that the Single Overall Ranking version. All of these observations are in consistence with the intuitive assumptions from the Methodology section.

Table 1 provides an overall summary of the experiments carried out. It can be seen that all of the experiments were carried out on optimally trained networks. The percentages shown represent the amount of pruning possible without a significant drop in performance.

In conclusion, it can be said that using the second-order Taylor Series expansion of the error function to rank individual neurons is an encouragingly accurate method of pruning networks to save memory. However it is definitely not the most accurate representation of the ranking based on the actual contribution of neurons to the error function. Another key take-away is that there are dependencies between individual neurons which might not be apparent from the outside. The better success of the Iterative Re-Ranking algorithm validates this. Perhaps a different approach like using Legendre Polynomials instead of the Taylor Series expansion would result in a better approximation of the neuron contributions.

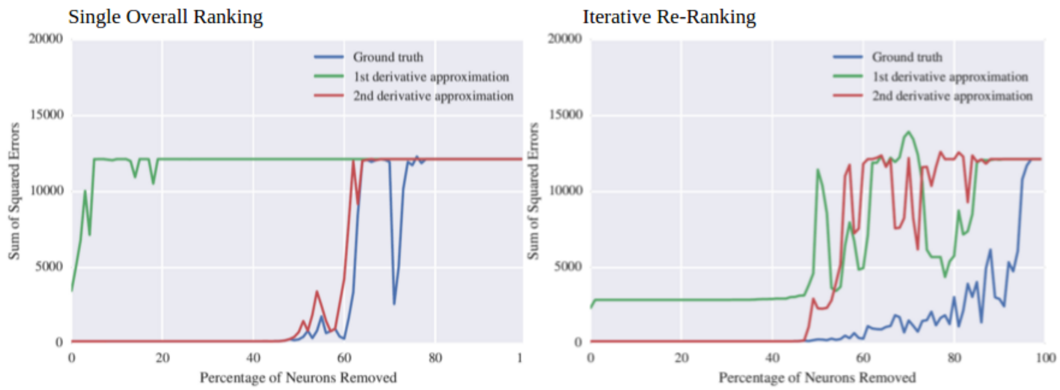

Figure 3: Performance on a diamond pattern dataset for both variations of the proposed algorithm. The blue curve shows the ground truth estimated from brute force pruning, the green and the red curves show pruning based on the approximation from first and second-order expansion of the Taylor Series.

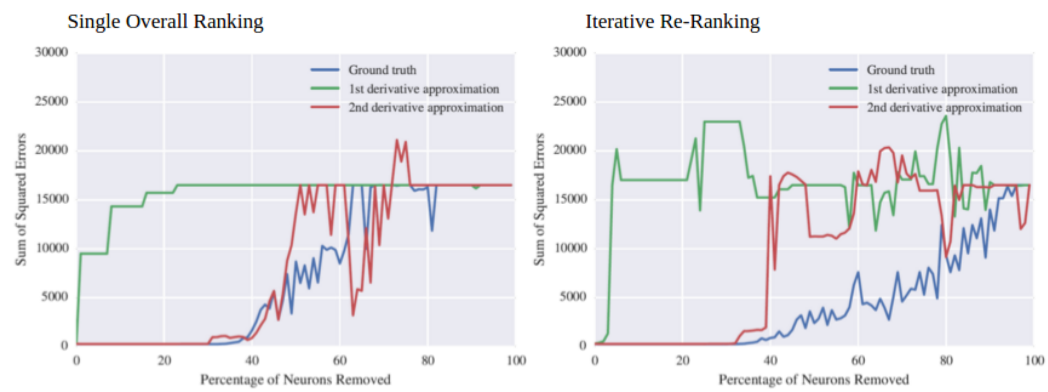

Figure 4: Performance on a random shape pattern dataset for both variations of the proposed algorithm. The blue curve shows the ground truth estimated from brute force pruning, the green and the red curves show pruning based on the approximation from first and second-order expansion of the Taylor Series.

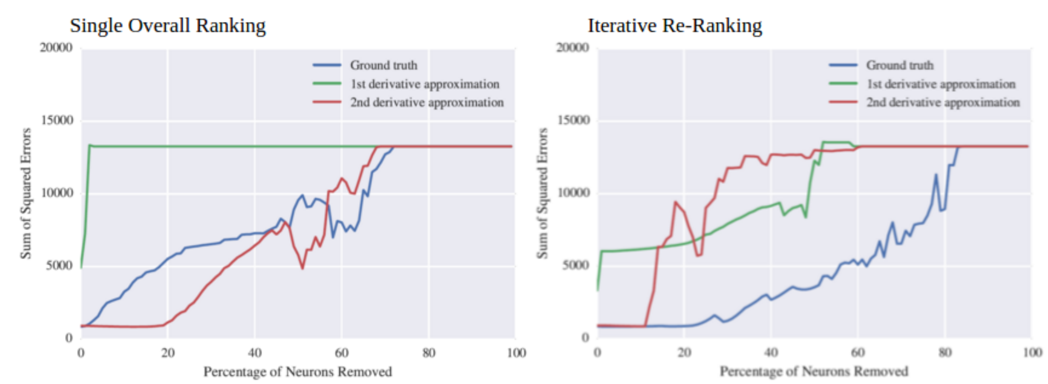

Figure 5: Performance on a distributed random shape pattern dataset for both variations of the proposed algorithm. The blue curve shows the ground truth estimated from brute force pruning, the green and the red curves show pruning based on the approximation from first and second-order expansion of the Taylor Series.

Pattern	Test Acc.	Ground Truth	Proposed Algorithm
Cosine Wave	0.9999	90%	70%
Diamond	0.9921	48%	48%
Random	0.9861	38%	35%
Dist. Random	0.9601	20%	10%
Circle	0.9968	40%	0%

Table 1: A comparison of the percentage pruning achieved using brute force and the proposed algorithm on optimally trained networks. The percentages shown represent the amount of pruning possible without a significant drop in performance.

4 COSINE FUNCTION

5 DISCUSSION OF RESULTS

* first or second layer? * cascade correlation in reverse? * retraining? * investigation of the true independence of the elements

6 Appendix A: Second Derivative Back-Propagation

Name and network definitions:

$$E = \frac{1}{2}\sum_i (o_i^{(0)} - t_i)^2 \quad o_i^{(m)} = \sigma(x_i^{(m)}) \quad x_i^{(m)} = \sum_j w_{ji}^{(m)} o_j^{(m+1)} \quad c_{ji}^{(m)} = w_{ji}^{(m)} o_j^{(m+1)} \tag{1}$$

Superscripts represent the index of the layer of the network in question, with 0 representing the output layer. E is the squared-error network cost function. $o_i^{(m)}$ is the ith output in layer m generated by the activation function σ, which in this paper is is the standard logistic sigmoid. $x_i^{(m)}$ is the weighted sum of inputs to the ith neuron in the mth layer, and $c_{ji}^{(m)}$ is the contribution of the jth neuron in the $m+1$ layer to the input of the ith neuron in the mth layer.

6.1 First and Second Derivatives

The first and second derivatives of the cost function with respect to the outputs:

$$\frac{\partial E}{\partial o_i^{(0)}} = o_i^{(0)} - t_i \tag{2}$$

$$\frac{\partial^2 E}{\partial {o_i^{(0)}}^2} = 1 \tag{3}$$

The first and second derivatives of the sigmoid function in forms depending only on the output:

$$\sigma'(x) = \sigma(x)\,(1 - \sigma(x)) \tag{4}$$
$$\sigma''(x) = \sigma'(x)\,(1 - 2\sigma(x)) \tag{5}$$

The second derivative of the sigmoid is easily derived from the first derivative:

$$\sigma'(x) = \sigma(x)\,(1 - \sigma(x)) \tag{6}$$
$$\sigma''(x) = \frac{\mathrm{d}}{\mathrm{d}x} \underbrace{\sigma(x)}_{f(x)} \underbrace{(1 - \sigma(x))}_{g(x)} \tag{7}$$
$$\sigma''(x) = f'(x)g(x) + f(x)g'(x) \tag{8}$$
$$\sigma''(x) = \sigma'(x)(1 - \sigma(x)) - \sigma(x)\sigma'(x) \tag{9}$$
$$\sigma''(x) = \sigma'(x) - 2\sigma(x)\sigma'(x) \tag{10}$$
$$\sigma''(x) = \sigma'(x)(1 - 2\sigma(x)) \tag{11}$$

And for future convenience:

$$\frac{\mathrm{d}o_i^{(m)}}{\mathrm{d}x_i^{(m)}} = \frac{\mathrm{d}}{\mathrm{d}x_i^{(m)}} \left(o_i^{(m)} = \sigma(x_i^{(m)}) \right) \tag{12}$$
$$= \left(o_i^{(m)}\right)\left(1 - o_i^{(m)}\right) \tag{13}$$
$$= \sigma'\left(x_i^{(m)}\right) \tag{14}$$
$$\frac{\mathrm{d}^2 o_i^{(m)}}{\mathrm{d}{x_i^{(m)}}^2} = \frac{\mathrm{d}}{\mathrm{d}x_i^{(m)}} \left(\frac{\mathrm{d}o_i^{(m)}}{\mathrm{d}x_i^{(m)}} = \left(o_i^{(m)}\right)\left(1 - o_i^{(m)}\right) \right) \tag{15}$$
$$= \left(o_i^{(m)}\left(1 - o_i^{(m)}\right)\right)\left(1 - 2o_i^{(m)}\right) \tag{16}$$
$$= \sigma''\left(x_i^{(m)}\right) \tag{17}$$

Derivative of the error with respect to the ith neuron's input $x_i^{(0)}$ in the output layer:

$$\frac{\partial E}{\partial x_i^{(0)}} = \frac{\partial E}{\partial o_i^{(0)}} \frac{\partial o_i^{(0)}}{\partial x_i^{(0)}} \tag{18}$$

$$= \underbrace{\left(o_i^{(0)} - t_i\right)}_{\text{from (2)}} \underbrace{\sigma\left(x_i^{(0)}\right)\left(1 - \sigma\left(x_i^{(0)}\right)\right)}_{\text{from (4)}} \tag{19}$$

$$= \left(o_i^{(0)} - t_i\right)\left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right) \tag{20}$$

$$= \left(o_i^{(0)} - t_i\right)\sigma'\left(x_i^{(0)}\right) \tag{21}$$

Second derivative of the error with respect to the ith neuron's input $x_i^{(0)}$ in the output layer:

$$\frac{\partial^2 E}{\partial {x_i^{(0)}}^2} = \frac{\partial}{\partial x_i^{(0)}}\left(\frac{\partial E}{\partial o_i^{(0)}}\frac{\partial o_i^{(0)}}{\partial x_i^{(0)}}\right) \tag{22}$$

$$= \frac{\partial^2 E}{\partial x_i^{(0)} \partial o_i^{(0)}}\frac{\partial o_i^{(0)}}{\partial x_i^{(0)}} + \frac{\partial E}{\partial o_i^{(0)}}\frac{\partial^2 o_i^{(0)}}{\partial {x_i^{(0)}}^2} \tag{23}$$

$$= \frac{\partial^2 E}{\partial x_i^{(0)} \partial o_i^{(0)}} \underbrace{\left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right)}_{\text{from (4)}} + \underbrace{\left(o_i^{(0)} - t_i\right)}_{\text{from (2)}} \underbrace{\left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right)\left(1 - 2o_i^{(0)}\right)}_{\text{from (5)}} \tag{24}$$

$$\left(\frac{\partial^2 E}{\partial x_i^{(0)} \partial o_i^{(0)}}\right) = \frac{\partial}{\partial x_i^{(0)}}\frac{\partial E}{\partial o_i^{(0)}} = \frac{\partial}{\partial x_i^{(0)}}\underbrace{\left(o_i^{(0)} - t_i\right)}_{\text{from (2)}} = \frac{\partial o_i^{(0)}}{\partial x_i^{(0)}} = \underbrace{\left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right)}_{\text{from (4)}} \tag{25}$$

$$\frac{\partial^2 E}{\partial {x_i^{(0)}}^2} = \left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right)^2 + \left(o_i^{(0)} - t_i\right)\left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right)\left(1 - 2o_i^{(0)}\right) \tag{26}$$

$$= \left(\sigma'\left(x_i^{(0)}\right)\right)^2 + \left(o_i^{(0)} - t_i\right)\sigma''\left(x_i^{(0)}\right) \tag{27}$$

First derivative of the error with respect to a single input contribution $c_{ji}^{(0)}$ from neuron j to neuron i with weight $w_{ji}^{(0)}$ in the output layer:

$$\frac{\partial E}{\partial c_{ji}^{(0)}} = \frac{\partial E}{\partial o_i^{(0)}}\frac{\partial o_i^{(0)}}{\partial x_i^{(0)}}\frac{\partial x_i^{(0)}}{\partial c_{ji}^{(0)}} \tag{28}$$

$$= \underbrace{\left(o_i^{(0)} - t_i\right)}_{\text{from (2)}} \underbrace{\left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right)}_{\text{from (4)}} \frac{\partial x_i^{(0)}}{\partial c_{ji}^{(0)}} \tag{29}$$

$$\left(\frac{\partial x_i^{(m)}}{\partial c_{ji}^{(m)}}\right) = \frac{\partial}{\partial c_{ji}^{(m)}}\left(x_i^{(m)} = \sum_j w_{ji}^{(m)} o_j^{(m+1)}\right) = \frac{\partial}{\partial c_{ji}^{(m)}}\left(c_{ji}^{(m)} + k\right) = 1 \tag{30}$$

$$\frac{\partial E}{\partial c_{ji}^{(0)}} = \left(o_i^{(0)} - t_i\right)\left(o_i^{(0)}\left(1 - o_i^{(0)}\right)\right) \tag{31}$$

$$= \underbrace{\left(o_i^{(0)} - t_i\right)\sigma'\left(x_i^{(0)}\right)}_{\text{from (21)}} \tag{32}$$

$$\frac{\partial E}{\partial c_{ji}^{(0)}} = \frac{\partial E}{\partial x_i^{(0)}} \tag{33}$$

Second derivative of the error with respect to a single input contribution $c_{ji}^{(0)}$:

$$\frac{\partial^2 E}{\partial {c_{ji}^{(0)}}^2} = \frac{\partial}{\partial c_{ji}^{(0)}} \left(\frac{\partial E}{\partial c_{ji}^{(0)}} = \underbrace{\left(o_i^{(0)} - t_i\right) \sigma'\left(x_i^{(0)}\right)}_{\text{from } (32)} \right) \tag{34}$$

$$= \frac{\partial}{\partial c_{ji}^{(0)}} \left(\sigma\left(x_i^{(0)}\right) - t_i\right) \sigma'\left(x_i^{(0)}\right) \tag{35}$$

$$= \frac{\partial}{\partial c_{ji}^{(0)}} \left(\sigma\left(\sum_j w_{ji}^{(m)} o_j^{(m+1)}\right) - t_i\right) \sigma'\left(\sum_j w_{ji}^{(m)} o_j^{(m+1)}\right) \tag{36}$$

$$= \frac{\partial}{\partial c_{ji}^{(0)}} \left(\sigma\left(\sum_j c_{ji}^{(0)}\right) - t_i\right) \sigma'\left(\sum_j c_{ji}^{(0)}\right) \tag{37}$$

$$= \frac{\partial}{\partial c_{ji}^{(0)}} \underbrace{\left(\sigma\left(c_{ji}^{(0)} + k\right) - t_i\right)}_{f\left(c_{ji}^{(0)}\right)} \underbrace{\sigma'\left(c_{ji}^{(0)} + k\right)}_{g\left(c_{ji}^{(0)}\right)} \tag{38}$$

We now make use of the abbreviations f and g:

$$= f'\left(c_{ji}^{(0)}\right) g\left(c_{ji}^{(0)}\right) + f\left(c_{ji}^{(0)}\right) g'\left(c_{ji}^{(0)}\right) \tag{39}$$

$$= \sigma'\left(c_{ji}^{(0)} + k\right) \sigma'\left(c_{ji}^{(0)} + k\right) + \left(\sigma\left(c_{ji}^{(0)} + k\right) - t_i\right) \sigma''\left(c_{ji}^{(0)} + k\right) \tag{40}$$

$$= \sigma'\left(c_{ji}^{(0)} + k\right)^2 + \left(o_i^{(0)} - t_i\right) \sigma''\left(c_{ji}^{(0)} + k\right) \tag{41}$$

$$\left(c_{ji}^{(0)} + k = \sum_j c_{ji}^{(0)} = \sum_j w_{ji}^{(m)} o_j^{(m+1)} = x_i^{(0)}\right) \tag{42}$$

$$\frac{\partial^2 E}{\partial {c_{ji}^{(0)}}^2} = \underbrace{\left(\sigma'\left(x_i^{(0)}\right)\right)^2 + \left(o_i^{(0)} - t_i\right) \sigma''\left(x_i^{(0)}\right)}_{\text{from } (27)} \tag{43}$$

$$\frac{\partial^2 E}{\partial {c_{ji}^{(0)}}^2} = \frac{\partial^2 E}{\partial {x_i^{(0)}}^2} \tag{44}$$

6.1.1 Summary Of Output Layer Derivatives

$$\frac{\partial E}{\partial o_i^{(0)}} = o_i^{(0)} - t_i \qquad \frac{\partial^2 E}{\partial {o_i^{(0)}}^2} = 1 \tag{45}$$

$$\frac{\partial E}{\partial x_i^{(0)}} = \left(o_i^{(0)} - t_i\right) \sigma'\left(x_i^{(0)}\right) \qquad \frac{\partial^2 E}{\partial {x_i^{(0)}}^2} = \left(\sigma'\left(x_i^{(0)}\right)\right)^2 + \left(o_i^{(0)} - t_i\right) \sigma''\left(x_i^{(0)}\right) \tag{46}$$

$$\frac{\partial E}{\partial c_{ji}^{(0)}} = \frac{\partial E}{\partial x_i^{(0)}} \qquad \frac{\partial^2 E}{\partial {c_{ji}^{(0)}}^2} = \frac{\partial^2 E}{\partial {x_i^{(0)}}^2} \tag{47}$$

6.1.2 Hidden Layer Derivatives

The first derivative of the error with respect to a neuron with output $o_j^{(1)}$ in the first hidden layer, summing over all partial derivative contributions from the output layer:

$$\frac{\partial E}{\partial o_j^{(1)}} = \sum_i \frac{\partial E}{\partial o_i^{(0)}} \frac{\partial o_i^{(0)}}{\partial x_i^{(0)}} \frac{\partial x_i^{(0)}}{\partial c_{ji}^{(0)}} \frac{\partial c_{ji}^{(0)}}{\partial o_j^{(1)}} = \sum_i \underbrace{\left(o_i^{(0)} - t_i\right) \sigma' \left(x_i^{(0)}\right)}_{\text{from } (21)} w_{ji}^{(0)} \tag{48}$$

$$\frac{\partial c_{ji}^{(m)}}{\partial o_j^{(m+1)}} = \frac{\partial}{\partial o_j^{(m+1)}} \left(c_{ji}^{(m)} = w_{ji}^{(m)} o_j^{(m+1)}\right) = w_{ji}^{(m)} \tag{49}$$

$$\frac{\partial E}{\partial o_j^{(1)}} = \sum_i \frac{\partial E}{\partial x_i^{(0)}} w_{ji}^{(0)} \tag{50}$$

Note that this equation does not depend on the specific form of $\frac{\partial E}{\partial x_i^{(0)}}$, whether it involves a sigmoid or any other activation function. We can therefore replace the specific indexes with general ones, and use this equation in the future.

$$\frac{\partial E}{\partial o_j^{(m+1)}} = \sum_i \frac{\partial E}{\partial x_i^{(m)}} w_{ji}^{(m)} \tag{51}$$

The second derivative of the error with respect to a neuron with output $o_j^{(1)}$ in the first hidden layer:

$$\frac{\partial^2 E}{\partial {o_j^{(1)}}^2} = \frac{\partial}{\partial o_j^{(1)}} \frac{\partial E}{\partial o_j^{(1)}} \tag{52}$$

$$= \frac{\partial}{\partial o_j^{(1)}} \sum_i \frac{\partial E}{\partial x_i^{(0)}} w_{ji}^{(0)} \tag{53}$$

$$= \frac{\partial}{\partial o_j^{(1)}} \sum_i \left(o_i^{(0)} - t_i\right) \sigma' \left(x_i^{(0)}\right) w_{ji}^{(0)} \tag{54}$$

If we now make use of the fact, that $o_i^{(0)} = \sigma\left(x_i^{(0)}\right) = \sigma\left(\sum_j \left(w_{ji}^{(0)} o_j^{(1)}\right)\right)$, we can evaluate the expression further.

$$\frac{\partial^2 E}{\partial {o_j^{(1)}}^2} = \frac{\partial}{\partial o_j^{(1)}} \sum_i \underbrace{\left(\sigma\left(\sum_j w_{ji}^{(0)} o_j^{(1)}\right) - t_i\right)}_{f\left(o_j^{(1)}\right)} \underbrace{\sigma'\left(\sum_j w_{ji}^{(0)} o_j^{(1)}\right) w_{ji}^{(0)}}_{g\left(o_j^{(1)}\right)} \tag{55}$$

$$= \sum_i \left(f'\left(o_j^{(1)}\right) g\left(o_j^{(1)}\right) + f\left(o_j^{(1)}\right) g'\left(o_j^{(1)}\right)\right) \tag{56}$$

$$= \sum_i \sigma'\left(\sum_j w_{ji}^{(0)} o_j^{(1)}\right) w_{ji}^{(0)} \, \sigma'\left(\sum_j w_{ji}^{(0)} o_j^{(1)}\right) w_{ji}^{(0)} + \ldots \tag{57}$$

$$\sum_i \left(\sigma\left(\sum_j w_{ji}^{(0)} o_j^{(1)}\right) - t_i\right) \sigma''\left(\sum_j w_{ji}^{(0)} o_j^{(1)}\right) \left(w_{ji}^{(0)}\right)^2 \tag{58}$$

$$= \sum_i \left(\left(\sigma'\left(x_i^{(0)}\right)\right)^2 \left(w_{ji}^{(0)}\right)^2 + \left(o_i^{(0)} - t_i\right) \sigma''\left(x_i^{(0)}\right) \left(w_{ji}^{(0)}\right)^2\right) \tag{59}$$

$$= \sum_i \underbrace{\left(\left(\sigma'\left(x_i^{(0)}\right)\right)^2 + \left(o_i^{(0)} - t_i\right) \sigma''\left(x_i^{(0)}\right)\right)}_{\text{from } (27)} \left(w_{ji}^{(0)}\right)^2 \tag{60}$$

Summing up, we obtain the more general expression:

$$\frac{\partial^2 E}{\partial {o_j^{(1)}}^2} = \sum_i \frac{\partial^2 E}{\partial {x_i^{(0)}}^2} \left(w_{ji}^{(0)}\right)^2 \tag{61}$$

Note that the equation in (61) does not depend on the form of $\frac{\partial^2 E}{\partial {x_x^{(0)}}^2}$, which means we can replace the specific indexes with general ones:

$$\frac{\partial^2 E}{\partial {o_j^{(m+1)}}^2} = \sum_i \frac{\partial^2 E}{\partial {x_i^{(m)}}^2} \left(w_{ji}^{(m)}\right)^2 \tag{62}$$

At this point we are beginning to see the recursion in the form of the 2nd derivative terms which can be thought of analogously to the first derivative recursion which is central to the back-propagation algorithm. The formulation above which makes specific reference to layer indexes also works in the general case.

Consider the ith neuron in any layer m with output $o_i^{(m)}$ and input $x_i^{(m)}$. The first and second derivatives of the error E with respect to this neuron's *input* are:

$$\frac{\partial E}{\partial x_i^{(m)}} = \frac{\partial E}{\partial o_i^{(m)}} \frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} \tag{63}$$

$$\begin{aligned}
\frac{\partial^2 E}{\partial {x_i^{(m)}}^2} &= \frac{\partial}{\partial x_i^{(m)}} \frac{\partial E}{\partial x_i^{(m)}} && (64)\\
&= \frac{\partial}{\partial x_i^{(m)}} \left(\frac{\partial E}{\partial o_i^{(m)}} \frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} \right) && (65)\\
&= \frac{\partial^2 E}{\partial x_i^{(m)} \partial o_i^{(m)}} \frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} + \frac{\partial E}{\partial o_i^{(m)}} \frac{\partial^2 o_i^{(m)}}{\partial {x_i^{(m)}}^2} && (66)\\
&= \frac{\partial}{\partial o_i^{(m)}} \left(\frac{\partial E}{\partial x_i^{(m)}} = \frac{\partial E}{\partial o_i^{(m)}} \frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} \right) \frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} + \frac{\partial E}{\partial o_i^{(m)}} \sigma'' \left(x_i^{(m)}\right) && (67)\\
&= \frac{\partial^2 E}{\partial {o_i^{(m)}}^2} \left(\frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} \frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} \right) + \frac{\partial E}{\partial o_i^{(m)}} \sigma'' \left(x_i^{(m)}\right) && (68)\\
\frac{\partial^2 E}{\partial {x_i^{(m)}}^2} &= \frac{\partial^2 E}{\partial {o_i^{(m)}}^2} \left(\sigma' \left(x_i^{(m)}\right)\right)^2 + \frac{\partial E}{\partial o_i^{(m)}} \sigma'' \left(x_i^{(m)}\right) && (69)
\end{aligned}$$

Note the form of this equation is the general form of what was derived for the output layer in (27). Both of the above first and second terms are easily computable and can be stored as we propagate back from the output of the network to the input. With respect to the output layer, the first and second derivative terms have already been derived above. In the case of the $m+1$ hidden layer during back propagation, there is a summation of terms calculated in the mth layer. For the first derivative, we have this from (51).

$$\frac{\partial E}{\partial o_j^{(m+1)}} = \sum_i \frac{\partial E}{\partial x_i^{(m)}} w_{ji}^{(m)} \tag{70}$$

And the second derivative for the jth neuron in the $m+1$ layer:

$$\frac{\partial^2 E}{\partial {x_j^{(m+1)}}^2} = \frac{\partial^2 E}{\partial {o_j^{(m+1)}}^2} \left(\sigma' \left(x_j^{(m+1)}\right)\right)^2 + \frac{\partial E}{\partial o_j^{(m+1)}} \sigma'' \left(x_j^{(m+1)}\right) \tag{71}$$

We can replace both derivative terms with the forms which depend on the previous layer:

$$\frac{\partial^2 E}{\partial {x_j^{(m+1)}}^2} = \underbrace{\sum_i \frac{\partial^2 E}{\partial {x_i^{(0)}}^2} \left(w_{ji}^{(0)}\right)^2}_{\text{from } (62)} \left(\sigma' \left(x_j^{(m+1)}\right)\right)^2 + \underbrace{\sum_i \frac{\partial E}{\partial x_i^{(m)}} w_{ji}^{(m)}}_{\text{from } (51)} \sigma'' \left(x_j^{(m+1)}\right) \tag{72}$$

And this horrible mouthful of an equation gives you a general form for any neuron in the jth position of the $m+1$ layer. Taking very careful note of the indexes, this can be more or less translated painlessly to code. You are welcome, world.

6.1.3 Summary Of Hidden Layer Derivatives

$$\frac{\partial E}{\partial o_j^{(m+1)}} = \sum_i \frac{\partial E}{\partial x_i^{(m)}} w_{ji}^{(m)} \qquad \frac{\partial^2 E}{\partial {o_j^{(m+1)}}^2} = \sum_i \frac{\partial^2 E}{\partial {x_i^{(m)}}^2} \left(w_{ji}^{(m)}\right)^2 \tag{73}$$

$$\frac{\partial E}{\partial x_i^{(m)}} = \frac{\partial E}{\partial o_i^{(m)}} \frac{\partial o_i^{(m)}}{\partial x_i^{(m)}} \tag{74}$$

$$\frac{\partial^2 E}{\partial {x_j^{(m+1)}}^2} = \frac{\partial^2 E}{\partial {o_j^{(m+1)}}^2} \left(\sigma'\left(x_j^{(m+1)}\right)\right)^2 + \frac{\partial E}{\partial o_j^{(m+1)}} \sigma''\left(x_j^{(m+1)}\right) \tag{75}$$

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