Optimal Brain Surgeon and General Network Pruning

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Abstract—We investigate the use of information from all second order derivatives of the error function to perform network pruning (i.e., removing unimportant weights from a trained network) in order to improve generalization, simplify networks, reduce hardware or storage requirements, increase the speed of further training, and in some cases enable rule extraction. Our method, Optimal Brain Surgeon (OBS), is significantly better than magnitude-based methods and Optimal Brain Damage, which often remove the wrong weights. OBS permits pruning of more weights than other methods (for the same error on the training set), and thus yields better generalization on test data. Crucial to OBS is a recursion relation for calculating the inverse Hessian matrix $H^{-1}$ from training data and structural information of the net. OBS permits a 76%, a 62%, and a 90% reduction in weights over backpropagation with weight decay on three benchmark MONK's problems. Of OBS, Optimal Brain Damage, and a magnitude-based method, only OBS deletes the correct weights from a trained XOR network in every case. Finally, whereas Sejnowski and Rosenberg used 18,000 weights in their NETtalk network, we used OBS to prune a network to just 1,560 weights, yielding better generalization.

I. INTRODUCTION

A central problem in machine learning and pattern recognition is to minimize the system complexity (description length, VC-dimension, etc.) consistent with the training data. In neural networks this regularization problem is often cast as minimizing the number of connection weights. Without such weight elimination overfitting problems and thus poor generalization will result. Conversely, if there are too few weights, the network might not be able to learn the training data.

If we begin with a trained network having too many weights, the questions then become: Which weights should be eliminated? How should the remaining weights be adjusted for best performance? How can such network pruning be done in a computationally efficient way?

One possible magnitude based method [3] eliminates weights that have the smallest magnitude. This simple, plausible idea unfortunately often leads to the elimination of the wrong weights — small weights can be necessary for low error. Optimal Brain Damage [6] uses the criterion of minimal increase in training error for weight elimination. For computational simplicity, OBD assumes that the Hessian matrix is diagonal; in fact, however, Hessians for every problem we have considered are strongly non-diagonal, and this leads OBD to eliminate the wrong weights. The method described here — Optimal Brain Surgeon (OBS) — accepts the criterion used by Le Cun et al., but makes no restrictive assumptions about the form of the network's Hessian. OBS thereby eliminates the correct weights. Moreover, unlike other methods, OBS does not demand (typically slow) retraining after the pruning of a weight.

II. OPTIMAL BRAIN SURGEON

In deriving our method we begin, as do Le Cun, Denker and Solla [6], by considering a network trained to a local minimum in error. The functional Taylor series of the error with respect to weights (or parameters, see below) is:

$$
\delta E = \left( \frac{\partial E}{\partial w} \right)^T \cdot \delta w + \frac{1}{2} \delta w^T \cdot H \cdot \delta w + O(\| \delta w \|^3) \quad (1)
$$

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where $H \equiv \partial^2 E / \partial w^2$ is the Hessian matrix (containing all second order derivatives) and the superscript $T$ denotes vector transpose. For a network trained to a local minimum in error, the first (linear) term vanishes: we also ignore the third and all higher order terms. Our goal is then to set one of the weights to zero (which we call $w_q$) to minimize the increase in error given by Eq. 1. Eliminating $w_q$ is expressed as $\delta w_q + w_q = 0$ or more generally:

$$e_q^T \cdot \delta w + w_q = 0$$

(2)

where $e_q$ is the unit vector in weight space corresponding to (scalar) weight $w_q$. Our goal is then to solve:

$$\min_q \{ \min_{\delta w} \left[ \frac{1}{2} \delta w^T \cdot H \cdot \delta w \right] \mid e_q^T \cdot \delta w + w_q = 0 \}$$

(3)

To solve Eq. 3 we form a Lagrangian from Eqs. 1 and 2:

$$L = \frac{1}{2} \delta w^T \cdot H \cdot \delta w + \lambda (e_q^T \cdot \delta w + w_q)$$

(4)

where $\lambda$ is a Lagrange undetermined multiplier. We take functional derivatives, employ the constraints of Eq. 2, and use matrix inversion to find that the optimal weight change and resulting change in error are:

$$\delta w = \frac{w_q}{[H^{-1}]_{qq}} \cdot H^{-1} \cdot e_q$$

(5)

$$L_q = \frac{1}{2} \frac{w_q^2}{[H^{-1}]_{qq}}$$

(6)

Note that neither $H$ nor $H^{-1}$ need be diagonal (as is assumed by Le Cun et al.); moreover, our method recalculates the magnitude of all the weights in the network, by Eq. 5. We call $L_q$ the “saliency” of weight $q$ – the increase in error that results when the weight is eliminated – a definition more general than Le Cun et al.’s, and which includes theirs in the special case of diagonal $H$. Thus we have the algorithm of Table 1.

Table 1: Optimal Brain Surgeon procedure

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>Train a “reasonably large” network to minimum error.</td>
</tr>
<tr>
<td>2</td>
<td>Compute $H^{-1}$.</td>
</tr>
<tr>
<td>3</td>
<td>Find the q that gives the smallest saliency $L_q = w_q^2/(2[H^{-1}]_{qq})$. If this candidate error increase is much smaller than $E$, then the qth weight should be deleted, and we proceed to step 4; otherwise go to step 5. (Other stopping criteria can be used too.)</td>
</tr>
<tr>
<td>4</td>
<td>Use the q from step 3 to update all weights (Eq. 5). Go to step 2.</td>
</tr>
<tr>
<td>5</td>
<td>No more weights can be deleted without large increase in $E$. (At this point it may be desir- able to retrain the network.)</td>
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Figure 1 illustrates the basic idea. The relative magnitudes of the error after pruning (before retraining, if any) depend upon the particular problem, but to second order obey: $E(\text{mag}) \geq E(\text{OBD}) \geq E(\text{OBS})$, which is the key to the superiority of OBS. In this example OBS and OBD lead to the elimination of the same weight (weight 1). In many cases, however, OBS will eliminate different weights than those eliminated by OBD (cf. Sect. Vb).
call our method Optimal Brain Surgeon because in addition to deleting weights, it calculates and changes the strengths of other weights without the need for gradient descent or other incremental re-training.

III. COMPUTING THE INVERSE HESSIAN

The difficulty appears to be step 2 in the OBS procedure, since inverting a matrix of thousands or millions of terms seems computationally intractable. In what follows we shall give a general derivation of the inverse Hessian for a fully trained neural network. It makes no difference whether it was trained by backpropagation, competitive learning, the Boltzmann algorithm, or any other method, so long as derivatives can be taken (see below). We shall show that the Hessian can be reduced to the sample covariance matrix associated with certain gradient vectors. Furthermore, the gradient vectors necessary for OBS are normally available at small computational cost; the covariance form of the Hessian yields a recursive formula for computing the inverse.

Consider a general non-linear neural network that maps an input vector, in, of dimension $n_i$ into an output vector, o, of dimension $n_o$, according to the following:

$$o = F(w, in)$$

(7)

where $w$ is an $n$-dimensional vector representing the neural network's weights or other parameters. We shall refer to $w$ as a weight vector below for simplicity and definiteness, but it must be stressed that $w$ could represent any continuous parameters, such as those describing neural transfer function, weight sharing, and so on. The mean square error on the training set is defined as:

$$E = \frac{1}{2P} \sum_{k=1}^{P} (t^{[k]} - o^{[k]})^T(t^{[k]} - o^{[k]})$$

(8)

where $P$ is the number of training patterns, and $t^{[k]}$ and $o^{[k]}$ are the desired response and network response for the $k$th training pattern. The first derivative with respect to $w$ is:

$$\frac{\partial E}{\partial w} = -\frac{1}{P} \sum_{k=1}^{P} \left( \frac{\partial F(w, in^{[k]})}{\partial w} \cdot (t^{[k]} - o^{[k]}) \right)$$

(9)

and the second derivative or Hessian is:

$$H \equiv \frac{1}{P} \sum_{k=1}^{P} \left[ \frac{\partial F(w, in^{[k]})}{\partial w} \cdot \frac{\partial F(w, in^{[k]})}{\partial w}^T - \frac{\partial^2 F(w, in^{[k]})}{\partial w^2} \cdot (t^{[k]} - o^{[k]}) \right]$$

(10)

Next we consider a network fully trained to a local minimum in error at $w^*$. Under this condition the network response $o^{[k]}$ will be close to the desired response $t^{[k]}$, and hence we neglect the term involving $(t^{[k]} - o^{[k]})$. Even late in pruning, when this error is not small for a single pattern, this approximation can be justified (see next Section). This simplification yields:

$$H = \frac{1}{P} \sum_{k=1}^{P} \frac{\partial F(w, in^{[k]})}{\partial w} \cdot \frac{\partial F(w, in^{[k]})}{\partial w}^T$$

(11)

If our network has just a single output, we may define the $n$-dimensional data vector $X^{[k]}$ of derivatives as:

$$X^{[k]} \equiv \frac{\partial F(w, in^{[k]})}{\partial w}$$

(12)

Thus Eq. 11 can be written as:

$$H = \frac{1}{P} \sum_{k=1}^{P} X^{[k]} \cdot X^{[k]T}$$

(13)

If instead our network has multiple output units, then $X$ will be an $n \times n_o$ matrix of the form:

$$X^{[k]} \equiv \frac{\partial F(w, in^{[k]})}{\partial w} = \frac{\partial F_i(w, in^{[k]})}{\partial w} = \left( \frac{\partial F_{i1}(w, in^{[k]})}{\partial w}, \ldots, \frac{\partial F_{in_o}(w, in^{[k]})}{\partial w} \right)$$

(14)

where $F_i$ is the $i$th component of $F$. Hence in this multiple output unit case Eq. 11 generalizes to:

$$H = \frac{1}{P} \sum_{k=1}^{P} \sum_{i=1}^{n_o} X_i^{[k]} \cdot X_i^{[k]T}$$

(15)

Equations 13 and 15 show that $H$ is the sample covariance matrix associated with the gradient variable $X$. Equation 13 also shows that for the single output case we can calculate the full Hessian by sequentially adding in successive "component" Hessians as:

$$H_{m+1} = H_m + \frac{1}{P} X^{[m+1]} \cdot X^{[m+1]T}$$

(16)

with $H_0 = \alpha I$ and $H_P = H$.

But Optimal Brain Surgeon requires the inverse of $H$ (Eq. 5). This inverse can be calculated using a standard matrix inversion formula [4]:

$$\begin{align*}
(A + B \cdot C \cdot D)^{-1} &= \left( A^{-1} - A^{-1} \cdot B \cdot (C^{-1} + D \cdot A^{-1} \cdot B)^{-1} \cdot D \cdot A^{-1} \right) 
\end{align*}$$

(17)
applied to each term in the analogous sequence in Eq. 17:

$$H_{m+1}^{-1} = H_m^{-1} - \frac{H_m^{-1} \cdot X^{[m+1]} \cdot X^{[m+1]^T} \cdot H_m^{-1}}{P + X^{[m+1]^T} \cdot H_m^{-1} \cdot X^{[m+1]}}$$ (18)

with $H_0^{-1} = \alpha^{-1} I$ and $H_0^{-1} = H_{-1}^{-1}$ and $\alpha (10^{-8} \leq \alpha \leq 10^{-4})$ a small constant needed to make $H_0^{-1}$ meaningful, and to which our method is not especially sensitive [2]. Actually, Eq. 18 leads to the calculation of the inverse of $(H + \alpha I)$, and this corresponds to the introduction of a penalty term $\alpha\|d \|^2$ in Eq. 4. This effective weight decay has the benefit of penalizing large candidate jumps in weight space, and thus helps to ensure that the neglecting of higher order terms in Eq. 1 is valid.

Equation 18 permits the calculation of $H^{-1}$ using a single sequential pass through the training data $1 \leq m \leq P$. It is also straightforward to generalize Eq. 19 to multiple outputs: in this case Eq. 16 is generalized to have recursions on both the indices $m$ and $l$ giving:

$$H_{m+1}^{-1} = H_m^{-1} + \frac{1}{P} X^{[m]} X^{[m]^T}$$  
$$H_{m+1} = H_m + \frac{1}{P} X^{[m]} X^{[m]^T}$$ (19)

To sequentially calculate $H^{-1}$ for the multiple output case, we use Eq. 17, as before.

IV. THE $(t-o) \to 0$ APPROXIMATION

The approximation used for Eq. 11 can be justified on computational and functional grounds, even late in pruning when the training error is not negligible. From the computational view, we note first that normally $H$ is degenerate – especially before significant pruning has been done – and its inverse not well defined. The approximation guarantees that there are no singularities in the calculation of $H^{-1}$. It also keeps the computational complexity of calculating $H^{-1}$ the same as that for calculating $H$. $O(Pn^2)$. In Statistics the approximation is the basis of Fisher’s method of scoring and its goal is to replace the true Hessian with its expected value and hence guarantee that $H$ is positive definite (thereby avoiding stability problems that can plague Gauss-Newton methods) [9].

Equally important are the functional justifications of the approximation. Consider a high capacity network trained to small training error. We can consider the network structure as involving both signal and noise. As we prune, we hope to eliminate those weights that lead to “overfitting,” i.e., learning the noise. If our pruning method did not employ the $(t-o) \to 0$ approximation, every pruning step (Eqs. 9 and 5) would inject the noise back into the system, by penalizing for noise terms. A different way to think of the approximation is the following. After some pruning by OBS we have reached a new weight vector that is a local minimum of the error (cf. Fig. 1). Even if this error is not negligible, we want to stay as close to that value of the error as we can. Thus we imagine a new, effective teaching signal $t^*$, that would keep the network near this new error minimum. It is then $(t^* - o)$ that we in effect set to zero when using Eq. 11 instead of Eq. 10.

V. OBS AND BACKPROPAGATION

Using the standard terminology from backpropagation [8] and the single output network of Fig. 2, it is straightforward to show from Eq. 12 that the derivative vectors are:

$$X^{[k]} = \begin{pmatrix} X^{[k]}_i \\ X^{[k]}_o \end{pmatrix}$$ (20)

where

$$[X^k]_i^T = (f'(...), f'(net^k_{[i]}),..., f'(net^k_{[i]}),...),$$ (21)

refers to derivatives with respect to hidden-to-output weights $w_{ji}$ and

$$[X^k]_o^T = (f'(...), f'(net^k_{[i]}),..., f'(net^k_{[i]}),...),$$ (22)

refers to derivatives with respect to input-to-hidden weights $u_{ij}$, and where lexicographical ordering has been used. The neuron nonlinearity is $f(\cdot)$.

Figure 2: Backpropagation net with $n_i$ inputs and $n_j$ hidden units. The input-to-hidden weights are $u_{ij}$ and hidden-to-output weights $r_j$. The derivative (“data”) vectors are $X_i$ and $X_o$ (Eqs. 20 and 21).
VI. Simulation results

We have found that OBS performs better than OBD and magnitude-based method on illustrative problems. We applied all three methods to the 2-2-1 network trained on the XOR problem. The network was first trained to a local minimum, which had zero error, and then each method was used to prune a single weight. Depending on the actual minimum found in the initial training, the three methods sometimes chose identical weights to prune, but oftentimes chose different weights. A typical run is shown in Fig. 3, where each of the methods has selected a different weight to be deleted. In this particular case, both OBD and the Magnitude based methods have made a fatal mistake: they have deleted a crucial weight, such that no amount of retraining can reduce the error back to 0. OBS on the other hand, never deletes such a crucial weight. In fact, in every case we observed, applying OBS to delete a weight and alter the remaining weights (Eq. 5) resulted in a networked that maintained perfect performance on the XOR problem. So, even in cases where the other pruning methods delete an incorrect weight (i.e. the resulting net can never relearn the problem), OBS provides a network which maintains perfect performance without any retraining by gradient descent.

Figure 4 shows the Hessian of the trained but unpruned XOR network of Fig. 3. It is clear that the off-diagonal terms do contribute significantly to the error of the network. This has been true of every problem we have looked at.

Figure 5 shows two-dimensional “slices” of the nine-dimensional error surface in the neighborhood of a local minimum at $w^*$ for the XOR network. The cuts compare the weight elimination the Magnitude method (left) and OBD (right) with the elimination and weight adjustment given by OBS. After pruning by OBS all network weights are updated by Eq. 5 and the system is at zero error (not shown).

It is especially noteworthy that for this error minimum $w^*$, the resulting networks after pruning by OBD or by the Magnitude method cannot achieve zero error, even after retraining. In short, magnitude methods and Optimal Brain Damage delete the wrong weights, and their mistake cannot be overcome by further network training. Only Optimal Brain Surgeon deletes the correct weight.

We also applied OBS to larger problems, three MONK’s problems, and compared our results to those of Thrun et al. [11]. whose backpropagation network outperformed all other approaches (network and rule-based) on these benchmark problems in an extensive machine learning competi-
tion. The Hessians for all three MONKs problems are far from diagonal.

Table 2 shows that for the same performance, OBS (without retraining) required only 24%, 38% and 10% of the weights of the backpropagation network, which was already regularized with weight decay (Fig. 6). The error increase $L$ (Eq. 5) accompanying pruning by OBS negligibly affected accuracy.

<table>
<thead>
<tr>
<th>MONK1</th>
<th>BPWD</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>training</td>
</tr>
<tr>
<td>BPWD</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>OBS</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>MONK2</td>
<td>BPWD</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>OBS</td>
<td>100</td>
</tr>
<tr>
<td>MONK3</td>
<td>BPWD</td>
<td>93.4</td>
</tr>
<tr>
<td></td>
<td>OBS</td>
<td>93.4</td>
</tr>
</tbody>
</table>

Table 2: The accuracy and number of weights determined by backpropagation with weight decay (BPWD) found by Thrun et al., and by OBS on three MONK’s problems.

The dramatic reduction in weights achieved by OBS yields a network that is simple enough that the logical rules that generated the data can be recovered from the pruned network, for instance by the methods of Towell and Shavlik [12]. Hence OBS may help to address a criticism often leveled at neural networks: the fact that they may be un-intelligible.

We applied OBS to a three-layer NETtalk network. While Sejnowski and Rosenberg [10] used 18,000 weights, we began with just 5,546 weights, which after backpropagation training had a sum-squared test error of 5,259. After pruning this net with OBS to 2,438 weights, and then retraining and pruning again, we achieved a net with only 1,560 weights and test error of only 4,701 – a significant improvement over the original, more complex network. Thus OBS can be applied to real-world pattern recognition problems such as speech recognition and optical character recognition, which typically have several thousand parameters.

VII. Analysis and conclusions

Why is Optimal Brain Surgeon so successful at reducing excess degrees of freedom? Conversely, given this new standard in weight elimination, we can ask: Why are the simplest magnitude based methods so poor? Consider again Fig. 1. Starting from the local minimum at $w^*$, a magnitude based method deletes the wrong weight, weight 2, and through retraining, weight 1 will increase. The final “solution” is weight 1 $\to$ large, weight 2 $\approx$ 0. This is precisely the opposite of the solution found by OBS: weight 1 $\approx$ 0, weight 2 $\to$ large. Although the actual difference in error shown in Fig. 1 may be small, in large networks differences from many incorrect weight elimination decisions can add up to a significant increase in error. But most importantly, it is simply wishful thinking to believe that after the elimination of many incorrect weights by magnitude methods the net can “sort it all out” through further training and reach a global optimum, especially if the network has already been pruned significantly (cf. XOR discussion, above).

We have also seen how the approximation employed by Optimal Brain Damage – that the diagonals of the Hessian are dominant – does not hold for the problems we have investigated. There are
typically many off-diagonal terms that are comparable or larger than their diagonal counterparts. This explains why OBD often deletes the wrong weight, while OBS deletes the correct one.

We note too that our method is quite general, and subsumes previous methods for weight elimination. In our terminology, magnitude based methods assume isotropic Hessian (H × I); OBD assumes diagonal H; FARM [5] assumes linear f(xw) and only updates the hidden-to-output weights. We have shown that none of those assumptions are valid nor sufficient for optimal weight elimination.

We should also point out that our method is even more general than presented here [2]. For instance, rather than pruning a weight (parameter) by setting it to zero, one can instead reduce a degree of freedom by projecting onto an arbitrary plane, e.g., \( w_0 = C \) a constant, though such networks typically have a large description length [7].

The pruning constraint \( w_0 = 0 \) discussed throughout this paper makes retraining (if desired) particularly simple. Several weights can be deleted simultaneously; bias weights can be exempt from pruning, and so forth. A slight generalization of OBS employs cross-entropy or the Kullback-Leibler error measure, leading to Fisher Information matrix rather than the Hessian [2]. We note too that OBS does not by itself give a criterion for when to stop pruning, and thus OBS can be utilized with a wide variety of such criteria. Moreover, gradual methods such as weight decay during learning can be used in conjunction with OBS.¹

REFERENCES


¹This is a revised and expanded version of Hassibi and Stork [1].