OPTIMIZATION TECHNIQUES FOR NEURAL NETWORKS

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TITLE PAGE

Optimization Techniques for Neural Networks

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Abstract

Parallelizable optimization techniques are applied to the problem of learning in feedforward neural networks. In addition to having superior convergence properties, optimization techniques such as the Polak-Ribiere method are also significantly more efficient than the Back-propagation algorithm. These results are based on experiments performed on small boolean learning problems and the noisy real-valued learning problem of hand-written character recognition.

1 INTRODUCTION

The problem of learning in feedforward neural networks has received a great deal of attention recently because of the ability of these networks to represent seemingly complex mappings in an efficient parallel architecture. This learning problem can be characterized as an optimization problem, but it is unique in several respects. Function evaluation is very expensive. However, because the underlying network is parallel in nature, this evaluation is easily parallelizable. In this paper, we describe the network learning problem in a numerical framework and investigate parallel algorithms for its solution. Specifically, we compare the performance of several parallelizable optimization techniques to the standard Back-propagation algorithm. Experimental results show the clear superiority of the numerical techniques.

2 Neural Networks

A neural network is characterized by its architecture. its node functions. and its interconnection weights. In a learning problem, the first two of these are fixed. so that the weight values are the only free parameters in the system. when we talk about "weight space" we refer to the parameter space defined by the weights in a network. thus a "weight vector" **w** is a vector or a point in weightspace which defines the values of each weight in the network. We will usually index the components of a weight vector as w_{ij}, meaning the weight value on the connection from unit i to unit j. Thus $\mathbf{N}(\mathbf{w}.\mathbf{r})$. a network function with n output units. is an n-dimensional vector-valued function defined for any weight vector **w** and any input vector **r**:

$$\mathbf{N}(\mathbf{w}.\mathbf{r}) = [o_1(\mathbf{w}.\mathbf{r}).o_2(\mathbf{w},\mathbf{r}),\ldots,o_n(\mathbf{w},\mathbf{r})]^T$$

where o_i is the i_{th} output unit of the network. Any node j in the network has input

$$i_j(\mathbf{w},\mathbf{r}) = \sum_{i \in \text{fanin}_j} o_i(\mathbf{w},\mathbf{r}) w_{ij}$$

and output

$$o_j(\mathbf{w},\mathbf{r}) = f_j(i_j(\mathbf{w},\mathbf{r})),$$

where $f_j()$ is the node function. There are various node functions in use but the one we shall concentrate on here is the "sigmoid" or *logistic* function:

$$f(x) = \frac{1}{1+e^{-x}}.$$

The evaluation of $\mathbf{N}()$ is inherently parallel and the time to evaluate $\mathbf{N}()$ on a single input vector is O(#layers). If pipelining is used, multiple input vectors can be evaluated in constant time.

3 Learning

The "learning" problem for a neural network refers to the problem of finding a network function which approximates some desired "target" function $\mathbf{T}()$. defined over the same set of input vectors as the network function. The problem is simplified by asking that the network function match the target function on only a finite set of input vectors. the "training set" R. This is usually done with an error measure. The most common measure is sum-squared error. which we use to define the "instance error" between $\mathbf{N}(\mathbf{w}.\mathbf{r})$ and $\mathbf{T}(\mathbf{r})$ at weight vector $\mathbf{w}$ and input vector $\mathbf{r}$:

$$e_{\mathbf{N}.\mathbf{T}}(\mathbf{w}.\mathbf{r}) = \sum_{i \in \text{outputs}} \tfrac{1}{2}(T_i(\mathbf{r}) - o_i(\mathbf{w}.\mathbf{r}))^2 = \tfrac{1}{2}\|\mathbf{T}(\mathbf{r}) - \mathbf{N}(\mathbf{w}.\mathbf{r})\|^2.$$

We can now define the "error function" between $\mathbf{N}()$ and $\mathbf{T}()$ over R as a function of $\mathbf{w}$:

$$E_{\mathbf{N}.\mathbf{T}.R}(\mathbf{w}) = \sum_{\mathbf{r} \in R} e_{\mathbf{N}.\mathbf{T}}(\mathbf{w}.\mathbf{r}).$$

The learning problem is thus reduced to finding a $\mathbf{w}$ for which $E_{\mathbf{N}.\mathbf{T}.R}(\mathbf{w})$ is minimized. If this minimum value is zero then the network function approximates the target function exactly on all input vectors in the training set. Henceforth. for notational simplicity we will write $e()$ and $E()$ rather than $e_{\mathbf{N}.\mathbf{T}}()$ and $E_{\mathbf{N}.\mathbf{T}.R}()$.

4 Optimization Techniques

As we have framed it here, the learning problem is a classic problem in optimization. More specifically, network learning is a problem of function approximation, where the approximating function is a finite parameter-based system. The goal is to find a set of parameter values which minimizes a cost function, which in this case, is a measure of the error between the target function and the approximating function.

Among the optimization algorithms that can be used to solve this type of problem. gradient-based algorithms have proven to be effective in a variety of applications {Avriel, 1976}. These algorithms are iterative in nature. thus $\mathbf{w}_k$ is the weight vector at the k_{th} iteration. Each iteration is characterized by a *search direction* $\mathbf{d}_k$ and a *step* α_k. The weight vector is updated by taking a *step* in the *search direction* as below:

```
for($k$=0; evaluate($\mathbf{w}_k$) != CONVERGED; ++$k$) {
  $\mathbf{d}_k$ = determine_search_direction();
  $\alpha_k$ = determine_step();
  $\mathbf{w}_{k+1}$ = $\mathbf{w}_k$ + $\alpha_k\mathbf{d}_k$;
}
```

If $\mathbf{d}_k$ is a direction of descent, such as the negative of the gradient, a sufficiently small step will reduce the value of $E()$. Optimization algorithms vary in the way they determine α and $\mathbf{d}$, but otherwise they are structured as above.

5 Convergence Criterion

The choice of convergence criterion is important. An algorithm must terminate when $E()$ has been sufficiently minimized. This may be done with a threshold on the value of $E()$, but this alone is not sufficient. In the case where the error surface contains "bad" local minima, it is possible that the error threshold will be unattainable, and in this case the algorithm will never terminate. Some researchers have proposed the use of an iteration limit to guarantee termination despite an unattainable error threshold {Fahlman, 1989}. Unfortunately, for practical problems where this limit is not known *a priori*, this approach is inapplicable.

A necessary condition for $\mathbf{w}^*$ to be a minimum, either local or global, is that the gradient $\mathbf{g}(\mathbf{w}^*) = \nabla E(\mathbf{w}^*) = 0$. Hence, the most usual convergence criterion for optimization algorithms is

$$||\mathbf{g}(\mathbf{w}_k)|| \leq \epsilon$$

where ϵ is a sufficiently small *gradient threshold*. The downside of using this as a convergence test is that, for successful trials, learning times will be longer than they would be in the case of an error threshold. Error tolerances are usually specified in terms of an acceptable bit error, and a threshold on the *maximum bit error (MBE)* is a more appropriate representation of this criterion than is a simple error threshold. The maximum bit error is the maximum individual output unit error over all outputs and over all training vectors:

$$MBE(\mathbf{w}_k) = \max_{\mathbf{r} \in R} \left(\max_{i \in \text{outputs}} \left(\tfrac{1}{2}(T_i(\mathbf{r}) - o_i(\mathbf{w}_k, \mathbf{r}))^2 \right) \right).$$

We have chosen a convergence criterion consisting of a gradient threshold and an MBE threshold (τ), terminating when

$$||\mathbf{g}(\mathbf{w}_k)|| \leq \epsilon \text{ or } MBE(\mathbf{w}_k) \leq \tau.$$

6 Steepest Descent

Steepest Descent is the most classical gradient-based optimization algorithm. In this algorithm the search direction $\mathbf{d}_k$ is always the negative of the gradient – the direction of steepest descent. For network learning problems the computation of $\mathbf{g}(\mathbf{w})$. the gradient of $E(\mathbf{w})$. is straightforward:

$$\mathbf{g}(\mathbf{w}) = \nabla E(\mathbf{w}) = \left[\frac{d}{d\mathbf{w}} \sum_{\mathbf{r}\in R} e(\mathbf{w},\mathbf{r})\right]^T = \sum_{\mathbf{r}\in R} \nabla e(\mathbf{w},\mathbf{r}).$$

where

$$\nabla e(\mathbf{w},\mathbf{r}) = \left[\frac{\partial e(\mathbf{w},\mathbf{r})}{\partial w_{11}}, \frac{\partial e(\mathbf{w},\mathbf{r})}{\partial w_{12}}, \ldots, \frac{\partial e(\mathbf{w},\mathbf{r})}{\partial w_{mn}}\right]^T.$$

$$\frac{\partial e(\mathbf{w},\mathbf{r})}{\partial w_{ij}} = o_i(\mathbf{w},\mathbf{r})\delta_j(\mathbf{w},\mathbf{r})$$

where for output units

$$\delta_j(\mathbf{w},\mathbf{r}) = f_j'(i_j(\mathbf{w},\mathbf{r}))(o_j(\mathbf{w},\mathbf{r}) - T_j(\mathbf{r})),$$

while for all other units

$$\delta_j(\mathbf{w},\mathbf{r}) = f_j'(i_j(\mathbf{w},\mathbf{r})) \sum_{k\in\mathrm{fanout}_j} \delta_k(\mathbf{w},\mathbf{r})w_{jk}.$$

The evaluation of $\mathbf{g}$ is thus almost dual to the evaluation of N; while the latter feeds forward through the net, the former feeds back. Both computations are inherently parallelizable and of the same complexity.

The method of Steepest Descent determines the step α_k by *inexact linesearch*, meaning that it minimizes

$$E(\mathbf{w}_k - \alpha_k\mathbf{d}_k).$$

There are many ways to perform this computation, but they are all iterative in nature and thus involve the evaluation of $E(\mathbf{w}_k - \alpha_k\mathbf{d}_k)$ for several values of α_k. As each evaluation requires a pass through the entire training set, this is expensive. *Curve fitting* techniques are employed to reduce the number of iterations needed to terminate a linesearch. Again, there are many ways to curve fit . We have employed the method of *false position* and used the *Wolfe Test* to terminate a linesearch {Luenberger, 1986}. In practice we find that the typical linesearch in a network learning problem terminates in 2 or 3 iterations.

7 Partial Conjugate Gradient Methods

Because linesearch guarantees that $E(\mathbf{w}_{k+1}) < E(\mathbf{w}_k)$, the Steepest Descent algorithm can be proven to converge for a large class of problems {Luenberger, 1986}. Unfortunately, its convergence rate is only linear and it suffers from the problem of "cross-stitching" {Luenberger, 1986}, so it may require a large number of iterations. One way to guarantee a faster convergence rate is to make use of higher order derivatives. Others have investigated the performance of algorithms of this class on network learning tasks, with mixed results {Becker, 1989}. We are not interested in such techniques because they are less parallelizable than the methods we have pursued and because they are more expensive, both computationally and in terms of storage requirements. Because we are implementing our algorithms on the Connection Machine, where memory is extremely limited, this last concern is of special importance. We thus confine our investigation to algorithms that require explicit evaluation only of $\mathbf{g}$, the first derivative.

Conjugate gradient techniques take advantage of second order information to avoid the problem of cross-stitching without requiring the estimation and storage of the Hessian (matrix of second-order partials). The search direction is a combination of the current gradient and the previous search direction:

$$\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k.$$

There are various rules for determining β_k; we have had the most success with the Polak-Ribiere rule, where β_k is determined from $\mathbf{g}_{k+1}$ and $\mathbf{g}_k$ according to

$$\beta_k = \frac{(\mathbf{g}_{k+1} - \mathbf{g}_k)^T \cdot \mathbf{g}_{k+1}}{\mathbf{g}_k^T \cdot \mathbf{g}_k}.$$

As in the Steepest Descent algorithm, α_k is determined by linesearch. With a simple reinitialization procedure partial conjugate gradient techniques are as robust as the method of Steepest Descent {Powell, 1977}; in practice we find that the Polak-Ribiere method requires far fewer iterations than Steepest Descent.

8 Back-propagation

The Batch Back-propagation algorithm {Rumelhart, 1986} can be described in terms of our optimization framework. Without momentum, the algorithm is very similar to the method of Steepest Descent in that

$$\mathbf{d}_k = -\mathbf{g}_k.$$

Rather than being determined by a linesearch, α, the "learning rate", is a fixed user-supplied constant. With momentum, the algorithm is similar to a partial conjugate gradient method, as

$$\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k$$

, though again β, the "momentum term", is fixed. On-line Back-propagation is a variation which makes a change to the weight vector following the presentation of each input vector:

$$\mathbf{d}_k = \nabla e(\mathbf{w}_k, \mathbf{r}_k).$$

Though very simple, we can see that this algorithm is numerically unsound for several reasons. Because β is fixed, $\mathbf{d}_k$ may not be a descent direction, and in this case any α will increase $E()$. Even if $\mathbf{d}_k$ is a direction of descent (as is the case for Batch Back-propagation without momentum), α may be large enough to move from one wall of a "valley" to the opposite wall, again resulting in an increase in $E()$. Because the algorithm can not guarantee that $E()$ is reduced by successive iterations, it cannot be proven to converge. In practice, finding a value for α which results in fast progress and stable behavior is a black art, at best.

9 Weight Decay

One of the problems of performing gradient descent on the "error surface" is that minima may be at infinity. (In fact, for boolean learning problems all minima are at infinity.) Thus an algorithm may have to travel a great distance through weightspace before it converges. Many researchers have found that weight decay is useful for reducing learning times {Hinton, 1986}. This technique can be viewed as adding a term corresponding to the length of the weight vector to the cost function: this modifies the cost surface in a way that bounds all the minima. Rather than minimizing on the error surface, minimization is performed on the surface with cost function

$$C(\mathbf{w}) = E(\mathbf{w}) + \frac{\gamma}{2}\|\mathbf{w}\|^2$$

where γ, the relative weight cost, is a problem-specific parameter. The gradient for this cost function is

$$\mathbf{g}(\mathbf{w}) = \nabla C(\mathbf{w}) = \nabla E(\mathbf{w}) + \gamma\mathbf{w},$$

and for any step α_k, the effect of γ is to "decay" the weight vector by a factor of $(1 - \alpha_k\gamma)$:

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \alpha_k\mathbf{g}_k = \mathbf{w}_k(1 - \alpha_k\gamma) - \alpha_k\nabla E(\mathbf{w}_k).$$

10 Parallel Implementation Issues

We have emphasized the parallelism inherent in the evaluation of $E()$ and $\mathbf{g}()$. To be efficient, any learning algorithm must exploit this parallelism. Without momentum, the Back-propagation algorithm is the simplest gradient descent technique, as it requires the storage of only a single vector, $\mathbf{g}_k$. Momentum requires the storage of only one additional vector, $\mathbf{d}_{k-1}$. The Steepest Descent algorithm also requires the storage of only a single vector more than Back-propagation without momentum: $\mathbf{d}_k$, which is needed for linesearch. In addition to $\mathbf{d}_k$, the Polak-Ribiere method requires the storage of two additional vectors: $\mathbf{d}_{k-1}$ and $\mathbf{g}_{k-1}$. The additional storage requirements of the optimization techniques are thus minimal. The additional computational requirements are essentially those needed for linesearch – a single dot product and a single broadcast per iteration. These operations are parallelizable (log time on the Connection Machine) so the additional computation required by these algorithms is also minimal, especially since computation time is dominated by the evaluation of $E()$ and $\mathbf{g}()$. Both the Steepest Descent and Polak-Ribiere algorithms are easily parallelizable. We have implemented these algorithms, as well as Back-propagation, on a Connection Machine {Hillis, 1986}.

11 Experimental Results

We have compared the performance of the Polak-Ribiere (P-R). Steepest Descent (S-D), and Batch Back-propagation (B-B) algorithms on small boolean learning problems. In all cases we have found the Polak-Ribiere algorithm to be significantly more efficient than the others. All the problems we looked at were based on three-layer networks (1 hidden layer) using the logistic function for all node functions. Initial weight vectors were generated by randomly choosing each component from $(+r, -r)$. γ is the relative weight cost. and ϵ and τ define the convergence test. Learning times are measured in terms of epochs (sweeps through the training set). All Back-propagation trials used $\alpha = 1$ and $\beta = 0$: these values were found to work about as well as any others.

The n-m-n encoder problem has n inputs, m hidden units and n outputs. There are n 1-hot encoded input vectors and the desired output vectors are the same 1-hot encoding. The encoder problem is of interest because it is easily scaled and has no bad local minima (assuming sufficient hidden units: log(#inputs)). The following three graphs compare the performance of the Polak-Ribiere technique (P-R), Steepest Descent (S-D), and Back-Propagation (BP) on a single run of the 10-5-10 encoder problem in terms of E, MBE and $\|\mathbf{g}\|$. All three were begun from the same initial random weight vector chosen with $r = 1.0$ and a value of 0.001 was used for γ. Note that all the plots are log-log. In terms of error or bit-error, Polak-Ribiere offers about an order of magnitude improvement for this example. More striking is the comparison of gradients, where Polak-Ribiere is almost two orders of magnitude more efficient. Note the cross-stitching that can be seen on the gradient plot for the steepest descent method (D).

Table 1 summarizes the results of our experiments on encoder problems. Average convergence times (in #epochs) for 100 independent trials of all three algorithms are shown, both for MBE convergence (first 5 entries) and gradient convergence (second 5 entries). Standard deviations for all data were insignificant ($< 25\%$). The minimum MBE possible for this problem (defined with $\gamma = 0.001$) was about 0.006, which explains the sudden rise for all three algorithms with $\tau = 0.007$: satisfying this MBE convergence criterion essentially requires finding the exact minimum which is equivalent to satisfying a gradient convergence criterion. Besides the fact that Polak-Ribiere was most efficient everywhere, the significant thing to note from the data is the superior convergence properties of Polak-Ribiere in satisfying a gradient criterion. Polak-Ribiere converges to minima at a rate of about 35 iterations per decade of accuracy (ϵ) while Back-Propagation converges at a rate of over 5000 iterations per decade!.

Tight encoders are encoders on networks where the size of the hidden layer is exactly equal to log(#inputs). that is n-(log n)-n encoders. Scaling experiments were done on the tight encoder problem from the 2-1-2 encoder to the 32-5-32 encoder. The results are summarized in the final 5 lines of table 1. but the important thing to note is that all of the algorithms scale linearly and thus that the optimization techniques retain their superiority over Back-Propagation.

TABLE 1. Encoder Results

Encoder	*num*	*Parameter Values*				*Avg Epochs to Convergence*		
Problem	*trials*	r	γ	τ	ϵ	*P-R*	*S-D*	*B-B*
10-5-10	100	1.0	1e-3	**1e-1**	1e-8	63.71	109.06	196.93
10-5-10	100	1.0	1e-3	**5e-2**	1e-8	66.89	119.91	225.90
10-5-10	100	1.0	1e-3	**2e-2**	1e-8	71.27	142.31	299.55
10-5-10	100	1.0	1e-3	**1e-2**	1e-8	77.33	178.70	549.66
10-5-10	100	1.0	1e-3	**7e-3**	1e-8	104.70	431.43	3286.20
10-5-10	100	1.0	1e-3	0.0	**1e-4**	279.52	1490.00	13117.00
10-5-10	100	1.0	1e-3	0.0	**1e-5**	318.02	1787.00	19792.00
10-5-10	100	1.0	1e-3	0.0	**1e-6**	353.30	2265.00	24910.00
10-5-10	100	1.0	1e-3	0.0	**1e-7**	384.65	2503.00	30076.00
10-5-10	100	1.0	1e-3	0.0	**1e-8**	417.90	2863.00	35260.00
4-2-4	100	1.0	1e-3	0.1	1e-8	36.92	56.90	179.95
8-3-8	100	1.0	1e-3	0.1	1e-8	67.63	194.80	594.76
16-4-16	100	1.0	1e-3	0.1	1e-8	121.30	572.80	990.33
32-5-32	25	1.0	1e-3	0.1	1e-8	208.60	1379.40	1826.15
64-6-64	25	1.0	1e-3	0.1	1e-8	405.60	4187.30	> 10000

The parity problem is interesting because it is also easily scaled and its weightspace is known to contain bad local minima. In the case where the initial random weight vector is in the basin of attraction of a bad local minima. the MBE threshold can not be satisfied and to terminate. the algorithm must satisfy the gradient threshold. In these cases the bad convergence properties of the Back-Propagation algorithm are most evident.

Problems such as parity also raise the question of how to report learning times for a weight space which contains bad minima. Most researchers report only learning times of successful trials. At most, they report the percentage of unsuccessful trials without mentioning the number of epochs required to decide that a trial is unsuccessful. To allow comparison of algorithms on neural network learning problems, it is important that the research community agree upon a metric for measuring learning times which is meaningful even in weight spaces with bad local minima. We propose a measure which we call *expected epochs to solution* (EES). This measure makes sense, especially if one considers an algorithm with a restart procedure which is able to restart itself from a new random weight vector whenever its gets stuck in a bad local minima. EES is thus the expected number of epochs needed for such an algorithm to find a solution vector in the weight space.

If $P(h)$ is the probability that a randomly chosen weight vector is in the basin of attraction of a solution (a hit) and $P(m)$ is the probability that that a randomly chosen weight vector is in the basin of attraction of a bad local minimum (a miss), then to calculate EES we see that a trial requiring i restarts has probability $P(h)P(m)^i$. If $E(h)$ is the expected epoch count for a hit, and $E(m)$ is the expected epoch count for a miss, then the expected epoch count for this trial with i restarts is $E(h)+iE(m)$. EES is simply the accumulated expectation on trials with all possible numbers of restarts:

$$\begin{aligned}
EES &= \sum_{i=0}^{\infty} P(h)P(m)^i(E(h)+iE(m)) \\
&= P(h)E(h)\sum_{i=0}^{\infty} P(m)^i + P(h)E(m)\sum_{i=0}^{\infty} iP(m)^i \\
&= P(h)E(h)\frac{1}{1-P(m)} + P(h)E(m)\frac{P(m)}{(1-P(m))^2} \\
&= \frac{P(h)E(h)+P(m)E(m)}{P(h)}
\end{aligned}$$

EES can thus be estimated fram a set of non-restarting trails as the ratio of total epochs to successful trials.

The results of the parity experiments are summarized in table 2. Again, the optimization techniques were more efficient than Back-propagation. This fact is most evident in the case of bad trials. All trials used $r = 1$, $\gamma = 1e-4$, $\tau = 0.1$ and $\epsilon = 1e-8$. Back-propagation used $\alpha = 1$ and $\beta = 0$.

TABLE 2. Parity Results

Parity	*alg*	*num*	$\%_{succ}$	avg_{succ}	(s.d.)	avg_{uns}	(s.d.)	*EES*
2-2-1	P-R	100	72%	73	(43)	232	(54)	163
	S-D	100	80%	95	(115)	3077	(339)	864
	B-B	100	78%	684	(1460)	47915	(5505)	14197
4-4-1	P-R	100	61%	352	(122)	453	(117)	641
	S-D	100	99%	2052	(1753)	18512	(-)	2324
	B-B	100	71%	8704	(8339)	95345	(11930)	48430
8-8-1	P-R	16	50%	1716	(748)	953	(355)	2669
	S-D	6	-	>1e4		>1e4		>1e4
	B-B	2	-	>1e5		>1e5		>1e5

12 Real-World Learning Problems

One of the criticisms of batch-based gradient descent techniques is that, for large real-world, real-valued learning problems, they will be be much less efficient than On-line Back-propagation. The reasoning behind this criticism can be seen from the following example: consider a training set R_0 consisting of m distinct training examples, and consider a second training set R_n consisting of 2^n copies of R_0. That is, each of the m distinct input vectors in R_0 is repeated 2^n times in R_n. In this case E_{R_n} is simply $2^n E_{R_0}$ and ∇E_{R_n} is $2^n \nabla E_{R_0}$ although the time to evaluate ∇E_{R_n} is 2^n times that to evaluate ∇E_{R_0} because of the difference in training set sizes. It is clear in this case that a lot of computational effort is being wasted in evaluating ∇E_{R_n}.

On-line Back-propagation is a variation of Back-propagation which makes a small change to the weight vector following the presentation of *each individual* input vector. Assuming the vectors of R_n are arranged as a repeating sequence of the vectors in R_0, On-line Back-propagation will require the same number of vector presentations, whether the vectors are coming from R_n or R_0. Thus the learning from R_n will require $\frac{1}{2^n}$ of the number of complete passes through the training set as the learning from R_0 and the overall learning times for both problems will be identical.

This will not be so for Batch Back-propagation, which only makes a change to the weight vector following an entire pass through the training set. Assuming that the learning rates have been normalized so that the learning rate for the problem based on R_n is $\frac{1}{2^n}$ the learning rate for the problem based on R_0, Batch Back-propagation will take the same moves for both problems and will require the same number of passes through the training sets. Because $|R_n|$ is $2^n|R_0|$, the overall learning time for the problem based on R_n will be 2^n times that for the problem based on R_0.

The argument goes that for learning problems with training sets consisting of many noisy input vectors, the situation is similar to the one described above. Because optimization techniques are similar to Batch Back-propagation in that they require a pass through the entire training set to evaluate ∇E before any changes are made to the weight vector, it is possible that for problems of this class optimization techniques may be less efficient than On-line Back-propagation.

13 Incremental Learning

If we consider a learning problem based on a training set consisting of many noisy examples of each of a finite number of output classes, then one way to increase the efficiency of batch-based algorithms on this problem would be through incremental learning. The idea of an incremental learning paradigm is to break the learning of a large training set into successive increments. Given a large training set consisting 2^n noisy examples of each of m output classes, we could directly train a naive network (one with a random initial weight vector $\mathbf{w}_0$) on the entire training set. Alternatively, we could create a series of successively larger training sets. R_0 would contain 1 example of each output class. R_1 would contain R_0 plus another example of each output class, $R2$ would contain R_1 plus another 2 examples of each output class, etc... In general, R_i would contain R_{i-1} plus another 2^{i-1} examples of each output class. R_n would thus be our original training set consisting of 2^n examples of each output class. To perform incremental learning. we could now train a network on R_0 beginning from an initial weight vector $\mathbf{w}_0^{(0)}$ which is random. We could then use the resulting trained weight vector $\mathbf{w}_*^{(0)}$ as the initial weight vector for training on R_1: $\mathbf{w}_0^{(1)} = \mathbf{w}_*^{(0)}$. $\mathbf{w}_*^{(1)}$ would be the initial vector for training on R_2, etc... In general. we would have that

$$\mathbf{w}_0^{(i)} = \mathbf{w}_*^{(i-1)}.$$

There are several reasons to think this approach may be more efficient. If we consider a contrived. fully redundant training set such as the one we used to compare On-line to Batch Back-propagation. a training set which consists of the same m output examples repeated 2^n times. it is clear that this incremental learning paradigm solves the inefficiency of Batch Back-propagation. When we finish training on the smallest training set, R_0. the resulting weight vector. $\mathbf{w}_*^{(0)}$ is a solution to all the remaining incremental learning problems. and thus learning is complete.

For more realistic training sets which contain multiple noisy examples of the same output class, we must consider the learning problem from a slightly different perspective. A weight vector is a "solution" to a learning problem if it causes the network to correctly classify all (or most) of the examples in the training set. There are two ways in which weight vector can accomplish this:

Memorization - the weight vector effectively stores all of the input vectors. The weight values on each of the hidden units encodes one of the input vectors and the output units values are determined according to which of the hidden units (now acting as "input vector detectors") are active. The resulting network will be very good at classifying the training vectors, but not very good at classifying new vectors it has not been trained on.

Generalization - the weight vector effectively defines a feature set for encoding the input vectors. The weight values on each of the hidden units encodes a particular "feature" which may be part of multiple input vectors. The output units values are determined by the set of features detected by the hidden layer. If many different examples of the same output class activate the same feature set, there is reason to hope than new examples of that input class will also activate the same feature set and thus that the network will be effective at classifying new input vectors that it has not been trained on.

If $\mathbf{w}_*^{(i-1)}$, the solution to the learning problem based on R_{i-1}, is the result of memorization, then $\mathbf{w}_*^{(i-1)}$ is far from a solution to the learning problem based on a larger training set, R_i. If, however, $\mathbf{w}_*^{(i-1)}$ is the result of good generalization, then it should be close to a solution for the learning problem based on R_i. In this case, $\mathbf{w}_*^{(i)}$ should also the result of good generalization and so should be close to a solution for the learning problem based on R_{i+1}, etc...

Another way to view this idea is in terms of weight spaces. If we define W to be the weight space defined by a learning problem, then our incremental training sets define a series of weight spaces $W_0, W_1, \ldots$. If this series is converging, in the mathematical sense, to some limit W_∞, then there ought to be some N such that, for all $i > N$, $\mathbf{w}_*^{(i)}$, a solution vector in W_i, is a solution vector in W_∞. In this case, we would have reason to expect that the incremental learning paradigm would be effective at reducing learning time.

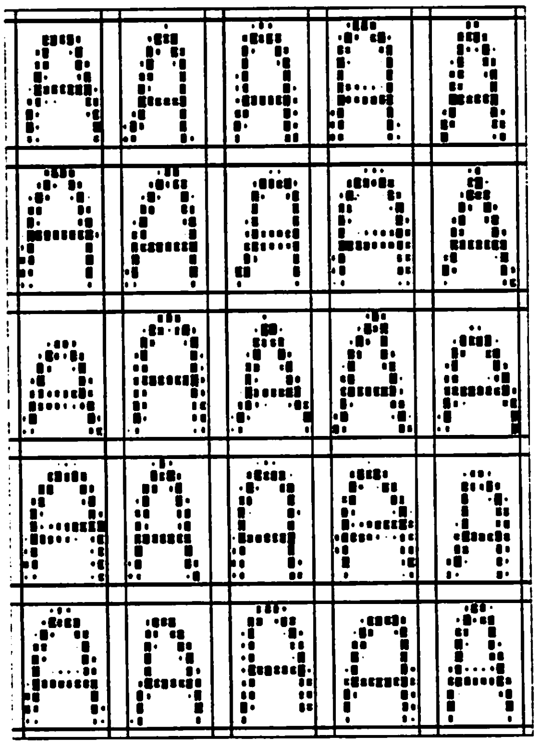
14 Letter Recognition

The task of characterizing hand drawn examples of the 26 capital letters was chosen as a good problem to compare the performance of gradient-based optimization techniques to On-line Back-propagation. This choice was made partly because others have used this problem to demonstrate that On-line Back-propagation is more efficient than Batch Back-propagation {Le Cun, 1986}. The experimental setup was as follows:

Characters were hand-entered in a 80×120 pixel window with a 5 pixel-wide brush (mouse controlled). Because the objective was to have many noisy examples of the same input pattern, not to learn scale and orientation invariance, all characters were roughly centered and roughly the full size of the window. Following character entry, the input window was symbolically gridded to define 100 8×12 pixel regions. Each of these regions was an input and the percentage of "on" pixels in the region was its value. There were thus 100 inputs, each of which could have any of 96 (8×12) distinct values. 26 outputs were used to represent a one-hot encoding of the 26 letters, and a network with a single hidden layer containing 10 units was chosen. The network thus had a 100-10-26 architecture; all nodes used the logistic function.

A training set consisting of 64 distinct sets of the 26 upper case letters was created by hand in the manner described. 25 "A" vectors are shown in figure 1. This large training set was recursively split in half to define a series of 6 successively larger training sets: R_0 to R_6, where R_0 is the smallest training set consisting of 1 of each letter and R_i contains R_{i-1} and 2^{i-1} new letter sets. A testing set consisting of 10 more sets of hand-entered characters was also created to measure network performance. For each R_i, we compared naive learning to incremental learning, where naive learning means initializing $\mathbf{w}_0^{(i)}$ randomly and incremental learning means setting $\mathbf{w}_0^{(i)}$ to $\mathbf{w}_*^{(i-1)}$ (the solution weight vector to the learning problem based on R_{i-1}). The incremental epoch count for the problem based on R_i was normalized to the number of epochs needed starting from $\mathbf{w}_*^{(i-1)}$ plus $\frac{1}{2}$ the number of epochs taken by the problem based on R_{i-1} (since $|R_{i-1}| = \frac{1}{2}|R_i|$). This normalized count thus reflects the total number of relative epochs needed to get from a naive network to a solution incrementally.

FIGURE 1 25 "A"s



Both Polak-Ribiere and On-line Back-propagation were tried on all problems; results are summarized in table 3. Only a single trial was done for each problem and all problems had $r = 1$, $\gamma = 0.01$, $\tau = 1e-8$ and $\epsilon = 0.1$. On-line Back-propagation was tried with $\alpha = 1.0$ and $\alpha = 0.1$ and in both cases β was 0. For On-line Back-propagation, γ was normalized to 0.01 divided by the trainingset size, thus giving an effective net γ of 0.01. Performance on the test set is shown in the last column.

TABLE 3. Letter Recognition

prob set	*Learning Time (epochs)*					*Test %*
	Polak-Ribiere			*On-line Back-prop*		
	INC	*NORM*	*NAIV*	$\alpha = 1.0$	$\alpha = 0.1$	
R0	92	92	92	267	2174	53.5
R1	55	120	78	135	1060	69.2
R2	31	90	104	69	579	80.4
R3	17	62	114	35	278	83.4
R4	109	140	160	21	192	92.3
R5	107	177	363	17	141	98.1
R6	46	134	684	500	7094	99.6

There are several things to note from the data. The first is that the incremental learning paradigm was very effective at reducing learning times. This is an indication that the solutions found show good generalization. In terms of epochs, the normalized learning times show a roughly constant learning time independent of problem size. This represents a learning time which is linearly dependent on the trainingset size in terms of real time. Larger problem sizes must be attempted to determine whether the downward trend on the largest problem continues. This would indicate that solutions to the smaller problems are solutions to the larger problems, so that little additional learning is required.

The On-line data is interesting as well. For many of the problems, learning time in terms of epochs is inversely proportional to trainingset size. This supports the claim that, for On-line Back-propagation, learning time depends only on number of input vector presentations, and is independent of the size of the training set from which they are being drawn. Unfortunately the learning time increases greatly for the largest problem (R6). This is true for both learning rates attempted. and while this increase has not been explained. it is an example of the instability inherent in this algorithm. The learning times for the On-line trials with $\alpha = 0.1$ are about ten times the learning times for the trials with $\alpha = 1.0$. This is an indication that the large increase on R6 was not due to a learning rate that was too large. Also. this data emphasizes the dependence of the performance of On-line Back-propagation on α. $\alpha = 10.0$ was tried but this learning rate was too high and resulted in oscillations and instability.

All that can be said in terms of a comparison of On-line Back-propagation and the Polak-Ribiere method from this data is that they appear to be in the same ballpark. Trials with larger problems must be made to make a more conclusive comparison of efficiency. The incremental leaning procedure appears to speed up Polak-Ribiere considerably. The other surprising result is that a network with only 10 hidden units was sufficient to solve this problem. indicating that these letters can be encoded by a compact set of features.

15 Conclusions

Describing the computational task of learning in feedforward neural networks as an optimization problem allows exploitation of the wealth of mathematical programming algorithms that have been developed over the years. We have found that the Polak-Ribiere algorithm offers superior convergence properties and significant speedup over the Batch Back-propagation algorithm. In addition. this algorithm is well-suited to parallel implementation on massively parallel computers such as the Connection Machine. Finally. incremental learning is a way to increase the efficiency of optimization techniques when applied to large real-world learning problems such as that of handwritten character recognition.

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