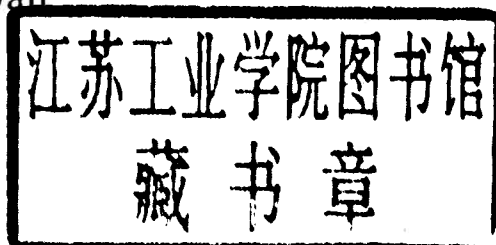


**2002 International Joint Conference
on Neural Networks
Vol. 1 (B)**

Proceedings of the
2002 International Joint Conference
on Neural Networks

IJCNN'02

May 12 – 17, 2002
Hilton Hawaiian Village Hotel
Honolulu, Hawaii



Co-sponsored by

Institute of Electrical and Electronics Engineers (IEEE)

IEEE Neural Networks Society (NNS)

International Neural Network Society (INNS)

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A MEMORY OPTIMAL BFGS NEURAL NETWORK TRAINING ALGORITHM

Seán F. McLoone, Vijanth S. Asirvadam and George W. Irwin
Intelligent Systems and Control Group
School of Electrical and Electronic Engineering
The Queen's University of Belfast
Ashby Building, Stranmillis Road, Belfast BT9 5AH, N. Ireland
Tel: (+44)(0)28 90 274535. Fax: (+44)(0)28 90 667023
Email: s.mcloone@ee.qub.ac.uk

Abstract- This paper considers the implementation of a novel memory optimal neural network training algorithm which maximises performance in relation to available memory. Mathematically it is similar to full memory (FM) BFGS (Broyden, Fletcher, Goldfarb and Shanno) training when there are no constraints on memory and to the variable memory (VM) BFGS when memory is limited. However, it requires less computations per iteration than VM and uses a much better strategy for discarding old curvature information when memory is limited.

I. INTRODUCTION

Off-line training of Multilayer Perceptrons (MLP) and feedforward neural networks has progressed considerably since the development of the batch backpropagation (BBP) algorithm [1]. The most significant advances have arisen from the exploitation of powerful, second-order methods from the field of unconstrained optimization. Contributions in this area include the scaled conjugate gradient (SCG) [2], memory-less (LM) BFGS [3], conjugate gradient with Powell restarts (CGPR) [4], Levenberg-Marquardt [5] and full memory (FM) BFGS training algorithms [6]. These training algorithms can be classified as being either matrix based or vector based according to whether their memory requirement are $O(N_w^2)$ or $O(N_w)$, where N_w is the number of network weights. Matrix based methods such as full memory BFGS and Levenberg-Marquardt, are two orders of magnitude faster than BBP, but at the expense of $O(N_w^2)$ memory usage. Vector based methods (e.g. conjugate gradient and memory-less BFGS) on the other hand use only a few vectors of storage ($O(N_w)$), but are not as powerful, being only one order of magnitude faster than BBP.

Available memory thus dictates the choice of training algorithm. In the past only two choices were possible; matrix based methods if sufficient memory was available; vector based techniques otherwise. Recently the authors proposed a third option, a variable memory (VM) BFGS training algorithm [7] based on the ideas of Buckley [8] and Nazareth [9], which bridges the gap between these two extremes. By storing cost function curvature information as a series of vectors rather than as a matrix this new algorithm is able to

optimize performance in relation to available memory. Numerically it has equivalent properties to FM BFGS when there are no memory restrictions and to FM BFGS with periodic reset when memory is limited. Achievable performance thus varies between that of matrix based and vector based methods as a function of the ratio between available memory and problem size.

This paper introduces an alternative memory optimal (OM) BFGS technique, based on the work of Nocedal [10], which has similar properties to VM BFGS, but requires less computations per iteration and uses a much better strategy for discarding old curvature information when memory is limited.

The paper is organized as follows. Section II gives an overview of some basic optimization theory and provides definition for the variables used throughout the paper. The standard full memory BFGS and memory-less BFGS are then briefly reviewed in section III. Section IV introduces variable memory (VM) BFGS and the new memory optimal (OM) alternative. Preliminary results are presented in section V comparing the new algorithm with the variable memory, full memory and memory less BFGS algorithms and finally section VI gives a summary and conclusions.

II. PRELIMINARIES

Training of feedforward neural networks can be viewed as an unconstrained optimization problem where the objective is to minimize a cost function $E(w)$, usually the sum-squared error over the training set, with respect to the network weights w . A Taylor's series expansion of $E(w)$ about the point w_0 gives

$$E(w) = E(w_0) + (w - w_0)^T g_0 + (w - w_0)^T H_0 (w - w_0) + \dots + \dots \quad (1)$$

where g_0 is the vector of gradients $\partial E / \partial w_i$ at w_0 and H_0 is the Hessian matrix of second-order derivatives, with elements:

$$h_{ij} = \frac{\partial^2 E}{\partial w_i \partial w_j} \quad (2)$$

Batch Back Propagation (BBP) training is based on a linear approximation to the actual error surface given by the first two terms in the Taylor series. i.e.,

$$E(\mathbf{w}) \approx E(\mathbf{w}_0) + (\mathbf{w} - \mathbf{w}_0)^T \mathbf{g}_0 \quad (3)$$

This approximation to $E(\mathbf{w})$ is a hyperplane, and as such does not have a minimum. However setting $\mathbf{w} = \mathbf{w}_0 - \eta \mathbf{g}_0$, where η is a positive scalar, does guarantee a reduction in error. Since the hyperplane approximation only holds for a very small region of $E(\mathbf{w})$ about $\mathbf{w}_0$, $E(\mathbf{w})$ only reduces for a small range of η , the best of which can be determined using a line-search [11].

The poor convergence properties of BBP can be attributed to the lack of accuracy of the search directions obtained from linear approximations to $E(\mathbf{w})$. Better performance can be expected if search directions are derived on the basis of a quadratic model of the error surface, that is,

$$E(\mathbf{w}) \approx E(\mathbf{w}_0) + (\mathbf{w} - \mathbf{w}_0)^T \mathbf{g}_0 + (\mathbf{w} - \mathbf{w}_0)^T H_0 (\mathbf{w} - \mathbf{w}_0) \quad (4)$$

Provided H_0 is positive definite this approximation has a global minimum at $\partial E / \partial \mathbf{w} = 0$ which is given by

$$\mathbf{w} = \mathbf{w}_0 - H_0^{-1} \mathbf{g}_0 \quad (5)$$

Since (4) is only a quadratic approximation to the actual cost function, $E(\mathbf{w})$, equation (5) can only be used as an estimate of the true minimum. Consequently an iterative approach has to be adopted where $-H^{-1} \mathbf{g}$ is used as a search direction in a similar manner to $-\mathbf{g}$ in BBP. Thus at each iteration $\mathbf{d}_k$ is given by

$$\mathbf{d}_k = -H_k^{-1} \mathbf{g}_k \quad (6)$$

This is known as Newton's search direction and is usually obtained by solving the system of linear equations

$$H_k \mathbf{d}_k = -\mathbf{g}_k \quad (7)$$

On well behaved cost functions Newton's algorithm converges *quadratically* to the minimum. However, in practice, cost functions are seldom well behaved with the result that in general H may not be positive definite or it may be ill-conditioned or even singular leading to premature termination. In addition the calculation of the inverse Hessian matrix is computationally very expensive ($O(N_w^3)$). Consequently Newton's method is seldom used directly. Instead alternative approaches have been developed which approximate Newton's search direction while avoiding direct calculation of the Hessian matrix. Some of these methods use approximations to the Hessian matrix or its inverse with built

in safeguards to maintain positive definiteness, while others make implicit use of Hessian information, thus avoiding its calculation completely. In the next section two such algorithms, Full Memory BFGS and memory-less BFGS, are described.

III. BFGS ALGORITHMS

A. Full Memory BFGS (FM)

Full memory (FM) BFGS belongs to the family of Quasi-Newton optimization methods. These are characterized by the fact that, instead of calculating H and then inverting it, the inverse of H is estimated directly by a symmetric positive definite matrix M which is updated iteratively in a manner which ensures positive definiteness and preservation of symmetry. The basic algorithm structure is as follow.

- Set the search direction ($\mathbf{d}_{k-1}$) equal to $-M_{k-1} \mathbf{g}_{k-1}$, where M_{k-1} is the approximation to H_{k-1}^{-1} at the $(k-1)^{\text{th}}$ iteration.
- Use a line search to find the weights which yield the minimum error along $\mathbf{d}_{k-1}$.

$$\mathbf{w}_k = \mathbf{w}_{k-1} + \eta_{opt} \mathbf{d}_{k-1} \quad (8)$$

$$\eta_{opt} = \min_{\eta} (E(\mathbf{w}_{k-1} + \eta \mathbf{d}_{k-1})) \quad (9)$$

- Compute the new gradient $\mathbf{g}_k$.
- Update the approximation to M_k using the new weight and gradient information.

$$\mathbf{s}_k = \mathbf{w}_k - \mathbf{w}_{k-1} \quad \text{and} \quad \mathbf{t}_k = \mathbf{g}_k - \mathbf{g}_{k-1} \quad (10)$$

$$A_k = \left(1 + \frac{\mathbf{t}_k^T M_{k-1} \mathbf{t}_k}{\mathbf{s}_k^T \mathbf{t}_k} \right) \frac{\mathbf{s}_k \mathbf{s}_k^T}{\mathbf{s}_k^T \mathbf{t}_k} \quad (11)$$

$$B_k = \frac{\mathbf{s}_k \mathbf{t}_k^T M_{k-1} + M_{k-1} \mathbf{t}_k \mathbf{s}_k^T}{\mathbf{s}_k^T \mathbf{t}_k} \quad (12)$$

$$M_k = M_{k-1} + A_k - B_k \quad (13)$$

The initial approximation to the inverse Hessian, M_0 , is normally taken as an identity matrix which corresponds to steepest descent (i.e. $\mathbf{d}_k = -\mathbf{g}_k$).

Matrices A, B and M are symmetric. This can be exploited so that only the lower triangle elements need to be computed and stored leading to a reduction of almost 50% in the computation complexity and memory requirements and facilitating partitioning of the update rule for parallel implementation [12].

FM BFGS is typically two orders of magnitude faster than the classical BBP, but this is achieved at the expense of

$O(N_w^2)$ computational complexity and memory usage. Consequently, while FM is very effective, it may not be feasible to use it to train neural networks with large numbers of weights ($N_w > 5000$).

B. Memory-Less BFGS (LM)

Memory-less BFGS [3] is a vector based training algorithm derived from FM BFGS. It is obtained by resetting M_{k-1} to the identity matrix in the BFGS update formulae (equation (13)) at each iteration and multiplying through by $-g_k$ to obtain a matrix free expression for the search direction

$$d_k = -g_k + a_k s_k + b_k t_k \quad (14)$$

$$a_k = -\left[1 + \frac{t_k^T t_k}{s_k^T t_k}\right] b_k + \frac{t_k^T g_k}{s_k^T t_k} \quad b_k = \frac{s_k^T g_k}{s_k^T t_k} \quad (15)$$

Memory-less BFGS has only $O(N_w)$ memory usage and computational complexity, but is also in general only one order of magnitude faster than BBP.

IV. MEMORY RESTRICTED BFGS

As discussed in the introduction, FM is a powerful training algorithm but because of $O(N_w^2)$ computation cost and memory requirements it cannot be used for large problems. LM or other $O(N_w)$ algorithms can be used instead, but at the expense of inferior performance. This leads to very poor utilization of resources, especially when the available memory is only marginally less than that required for FM. Clearly it would be desirable to have an algorithm that utilizes all available memory to maximise performance.

The weakness of FM can be attributed to the inefficient way in which it stores second-order curvature information. In the early stages of training matrix M contains only a small amount of information, yet storage is needed for all its elements. A much better strategy would be to store this information in a manner which ensures that memory requirements at a given iteration reflect the information content in the data store. This section will introduce two memory restricted BFGS algorithms which have this property.

A. Variable Memory BFGS (VM)

The BFGS update equation can be expressed in the form

$$M_k = M_{k-1} + \left[1 + \frac{v_k}{n_k}\right] \frac{s_k s_k^T}{n_k} - \frac{s_k u_k^T}{n_k} - \frac{u_k^T s_k}{n_k} \quad (16)$$

where

$$n_k = s_k^T t_k \quad u_k = M_{k-1} t_k \quad v_k = t_k^T u_k \quad (17)$$

In memory-less BFGS M_{k-1} is set to the identity matrix, I , and the expression is multiplied by the gradient to yield a matrix free expression for the search direction vector, d_k . A similar result can be achieved for the general case ($M_k \neq I$) by considering the multiplication of the BFGS update equation, (16), by an arbitrary vector r as follows.

$$M_k r = M_{k-1} r + \left[1 + \frac{v_k}{n_k}\right] \left[\frac{s_k^T r}{n_k}\right] s_k - \left[\frac{u_k^T r}{n_k}\right] s_k - \left[\frac{s_k^T r}{n_k}\right] u_k \quad (18)$$

This can be rewritten as

$$M_k r = M_{k-1} r - a_k(r) s_k - b_k(r) u_k \quad (19)$$

where $a_k(r)$ and $b_k(r)$ are scalars defined as

$$a_k(r) = \frac{u_k^T r}{n_k} - \left(1 + \frac{v_k}{n_k}\right) b_k(r) \quad b_k(r) = \frac{s_k^T r}{n_k} \quad (20)$$

$M_{k-1} r$ in equation (19) can be replaced by

$$M_{k-1} r = M_{k-2} r - a_{k-1}(r) s_{k-1} - b_{k-1}(r) u_{k-1} \quad (21)$$

and so on to give the general result

$$M_k r = M_{k-m} r - \sum_{j=k-m+1}^k (a_j(r) s_j + b_j(r) u_j) \quad (22)$$

where $m \leq k$. If the initial matrix M_0 is set to I , then selecting $m = k$ yields a matrix free expression for $M_k r$.

$$M_k r = r - \sum_{j=1}^k (a_j(r) s_j + b_j(r) u_j) \quad (23)$$

In order to compute this expression at the k^{th} iteration, the scalars v_j and n_j and vectors u_j and s_j have to be stored for all the previous iterations so that $a_j(r) s_j$ and $b_j(r) u_j$ can be determined for $j = 1$ to k . The current values of v_j , n_j and u_j are as defined in equation (17) with u_k computed using equation (23) with $r = t_k$, that is,

$$u_k = M_{k-1} t_k = t_k - \sum_{j=1}^{k-1} (a_j(t_k) s_j + b_j(t_k) u_j) \quad (24)$$

Using this result the FM search direction, $d_k = -M_k g_k$, can now be written in a matrix free variable memory (VM) form as

$$d_k = -g_k + \sum_{j=1}^k (a_j(g_k) s_j + b_j(g_k) u_j) \quad (25)$$

The memory requirements and computational complexity of VM BFGS increase linearly with iteration number and are