An Adaptive Memory Multi-Batch L-BFGS Algorithm for Neural Network Training

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Abstract: Motivated by the potential for parallel implementation of batch-based algorithms and the accelerated convergence achievable with approximated second order information a limited memory version of the BFGS algorithm has been receiving increasing attention in recent years for large neural network training problems. As the shape of the cost function is generally not quadratic and only becomes approximately quadratic in the vicinity of a minimum, the use of second order information by L-BFGS can be unreliable during the initial phase of training, i.e. when far from a minimum. Therefore, to control the influence of second order information as training progresses, we propose a multi-batch L-BFGS algorithm, namely MB-AM, that gradually increases its trust in the curvature information by implementing a progressive storage and use of curvature data through a development-based increase (dev-increase) scheme. Using six discriminative modelling benchmark problems we show empirically that MB-AM has slightly faster convergence and, on average, achieves better solutions than the standard multi-batch L-BFGS algorithm when training MLP and CNN models.

Keywords: Deep learning, L-BFGS, variable memory, quasi-Newton methods, neural networks

1. INTRODUCTION

In the last twenty years significant advances have been made towards making artificial neural networks able to compete with their biological counterparts (Dodge and Karam (2017)). A factor that is critical to the performance of artificial neural networks is the network training algorithm, which determines the sequence of computations to be performed in order for the network to learn the underlying relationships in the dataset of interest. Many training algorithms have been proposed over the years to achieve this goal, typically trading off computational complexity with rate-of-convergence and/or quality of solutions obtained (McLoone et al. (1998); Goodfellow et al. (2016); Ruder (2016)). In general, training algorithms fall into three categories: first order methods, which calculate the loss function and its derivative at each iteration, e.g. stochastic gradient descent (SGD) and Adam (Kingma and Ba (2014)), second order methods, which also calculate second derivative information, and quasi-Newton methods, which evaluate an approximation of the second derivative instead of computing it directly, e.g. the limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) (Liu and Nocedal (1989)). Whenever the amount of data to be processed is large, state-of-the-art performance is usually achieved with well-tuned first order methods thanks to regularization techniques such as batch normalization and dropout (Bollapragada et al. (2018)). Regularization and stable approximated curvature updates in L-BFGS methods are currently an active area of research due to the accelerated convergence achievable with curvature information and the ability to exploit parallelism with large batch sizes to achieve efficient algorithm implementations (Berahas et al. (2016); Yousefian et al. (2017)). Agarwal et al. (2014) proposed a hybrid approach where training is initially performed with a fast and regularized first order method and then switched to a full batch method to exploit parallelism. The L-BFGS method we propose can be seen as a hybrid approach where the batch size is kept fixed as in Berahas et al. (2016), but the use of approximated second order information is gradually increased during training thereby enhancing convergence. Initially, when little second order information is used, the method is essentially first order and becomes increasingly second order in nature as more and more curvature information is incorporated into the weight updates.

Our contributions: Motivated by recent interest in progressive training strategies (Smith et al. (2017); Bollapragada et al. (2018)), we propose an approach based on progressive curvature trust for the multi-batch L-BFGS algorithm of Berahas et al. (2016) by adding two algorithmic ingredients: a progressive storage (and use) of curvature information, and periodic resetting. Based on the development-based decay (dev-decay) scheme for first order methods (Wilson et al. (2017)), we propose a dev-increase scheme to control the progression of the memory size for curvature information and its resetting. For comparison purposes, we develop three variants of the multi-batch L-BFGS and experimentally compare them with the multi-batch L-BFGS and Adam algorithms for training.
multilayer perceptrons (MLPs) and convolutional neural networks (CNNs) on six case study datasets.

The paper is organized as follows: Section 2 describes the multi-batch L-BFGS algorithm of Berahas et al. (2016) as this is the reference algorithm to which we add two algorithmic ingredients; Section 3 explains the concept of \textit{progressive curvature trust} and the proposed algorithm; Section 4 describes the case studies and experiments conducted to evaluate the proposed algorithm and discusses the results obtained. Finally, Section 5 gives the conclusions.

Hereinafter, matrices and vectors are indicated with bold capital and bold lowercase letters, while lowercase italic font denotes scalars. The sets are indicated by italic capital and bold lowercase letters, while lowercase italic denotes scalars. The \textit{sets} are indicated by italic capital letters.

2. MULTI-BATCH L-BFGS

Let us consider a classification task defined by the set $B = \{x^{(i)}, l^{(i)} \}_{i=1, \ldots, |B|}$, where $x^{(i)} \in \mathbb{R}^n$ is an input sample (e.g. an image) of size $n$ and $l^{(i)} \in \mathbb{N}$ is an integer representing its class (i.e. label). A neural network relates the input to the output label via a mapping $p(\theta, x^{(i)}) : \mathbb{R}^n \rightarrow \mathbb{N}$, with network parameters $\theta \in \mathbb{R}^{d}$ optimally adapted to $B$ using a training algorithm. Full-batch algorithms learn the $\theta$ by considering the complete dataset $B$, therefore they optimize a deterministic function $C(B)$, that is

$$\min_\theta \frac{1}{|B|} \sum_{i \in B} c(x^{(i)}, l^{(i)}; p(\theta, x^{(i)})) = \min_\theta C(B),$$

where $c(\cdot)$ is a cost (i.e. loss) function chosen to measure the distance between the model prediction $\hat{l}^{(i)} = p(\theta, x^{(i)})$ and the expected output $l^{(i)}$ when given the sample $x^{(i)}$ as input. In contrast, in multi-batch mode a random subset $S_k \subset B$ is used at each iteration and the optimal $\theta$ is estimated by iteratively minimizing a stochastic cost function $C(S_k)$, that is

$$\min_{\theta_k} \frac{1}{|S_k|} \sum_{i \in S_k} c(x^{(i)}, l^{(i)}; p(\theta, x^{(i)})) = \min_{\theta_k} C(S_k), \tag{1}$$

where $k$ is the iteration counter. The L-BFGS algorithm updates the parameters with the rule

$$\theta_{k+1} = \theta_k - \eta H_k^{-1} g_k, \tag{2}$$

where $\eta$ is the learning rate (i.e. step length), $g_k$ is the gradient defined as

$$g_k = \frac{\partial C(S_k)}{\partial \theta_k} \tag{3}$$

and $H_k^{-1}$ is the inverse Hessian matrix approximation updated according to (Nocedal and Wright (2006))

$$H_{k+1}^{-1} = V_k^T H_k^{-1} V_k + \rho_k s_k s_k^T$$

$$p_k = (t_k^T s_k)^{-1}$$

$$V_k = I - \rho_k t_k s_k^T$$

$$s_k = \theta_{k+1} - \theta_k$$

$$t_k = g_k + s_k$$

The storage of $H_k^{-1}$ requires $O(d^2)$ memory, which is prohibitive with large neural networks, therefore in L-BFGS a two-loop recursion is used to directly compute the product $H_k^{-1} S_k$ such that only a predefined number of curvature pairs $(s_k, t_k)$ need to be stored. The maximum number of stored pairs, $m$, is usually fixed between 3 and 20 (Nocedal and Wright (2006)). Once the limit $m$ is reached the oldest pairs are replaced by the newest ones. Given the stochastic nature of the evaluation of the gradient using (3), to achieve a stable computation of the curvature $t_k$ (see (5)) Berahas et al. (2016) proposed having overlapping consecutive batches, i.e. $O_k = S_{k-1} \cap S_k \neq \emptyset$. This overlap is defined with the hyperparameter $\alpha = \frac{|O_k|}{|S_k|}$, which is usually chosen in the range $0 < \alpha < 0.5$.

3. ADAPTIVE MEMORY MULTI-BATCH L-BFGS

3.1 Local Approximation of the Cost Function

An important feature of gradient-based optimization algorithms is the computation of the search direction used to find an updated parameter vector $\theta_{k+1}$. Newton and quasi-Newton methods such as L-BFGS define the direction approximating the exact cost function $C$ with a quadratic model, obtained by truncating the cost function Taylor series expansion at the third term, that is:

$$C(\theta_k + y_k) \approx C_k = C(\theta_k) + g_k^T (\theta_k) y_k + \frac{1}{2} y_k^T H_k (\theta_k) y_k.$$  

Then, differentiating with respect to $y_k$ and setting it equal to zero we find the direction leading to the minimum of $C$

$$y_k = -H_k^{-1} g_k,$$

which motivates the weight update rule in (2). However, if around the point $\theta_k + y_k$ the function is significantly different from a quadratic-like model, the use of the curvature information could be detrimental to stable and reliable parameter updates. Moreover the curvature evaluation is computationally demanding as it requires the computation of $(d(d + 1))/2$ derivatives, thus it is only worth using if it actually improves the algorithm convergence.

Now we observe that as we approach a minimum point of a nonlinear multi-modal function the quadratic approximation becomes increasingly valid, and this occurs at the more advanced stages of training, i.e.

$$\lim_{k \to \infty} C - C_k = 0.$$  

In contrast, at the beginning of the training process it is difficult to say how well a quadratic model will approximate the true cost function.

Therefore, we propose an algorithm that implements a progressive use of curvature information: initially only a few curvature pairs (e.g. one or two) are stored and used, with the older pairs discarded to reduce the computational cost; then, when the algorithm gets closer to the minimum, we increase the storage and use of second order information.

3.2 The Algorithm

The pseudo-code of the proposed method is presented in Algorithm 1, which is the result of the combination of three building blocks:

\textbf{Block 1}: The basic structure is the multi-batch L-BFGS of Berahas et al. (2016) described in Section 2 which
performs stable curvature updates by overlapping consecutive batches. A PyTorch implementation is available on GitHub\(^1\).  

**Block 2:** To regulate the use of approximated second order information during training the memory \(m_k\) used to store the curvature pairs is increased as the number of iterations increases, in a fashion similar to the progressive batching approach proposed in Bollapragada et al. (2018). The rule defining when to increase \(m_k\) is based on the development of the validation loss in a similar fashion to the dev-decay scheme of Wilson et al. (2017) applied to the step length. Adapted to implement a progressive curvature trust, it becomes a dev-increase scheme. It is executed between Step 11 and Step 18, with α the increase of previous validation losses are stored and, if increased, a local minimum. The parameter \(m_{val}\) defines how many previous validation losses are stored and, if increased, makes the satisfaction of \(Q\) more difficult, thus delaying the increase of \(m_k\). The lower and upper limits of \(m_k\) are \(m_0\) and \(m_{max}\), respectively, i.e. \(m_0 \leq m_k \leq m_{max}\). Note that the extra memory required to store the validation losses is negligible with large datasets/models because \(m_{val}\) is a scalar and \(m_{val}\) is a relatively small number (e.g. \(m_{val} \leq \alpha\)).

\[
Q: \{\Delta_k-m_{val}+j > \Delta_{k-m_{val}+j+1}\}_{j=0,1,\ldots,m_{val}-2}
\]  
with \(\Delta_k = \|k-1 - v_k\).  

**Block 3:** To further mitigate the impact of using unrepresentative curvature information, the resetting of the memory proposed in McLoone and Irwin (1999) is implemented. Adapted to implement a progressive curvature trust, the resetting is applied just for smaller \(k\) according to the development of \(m_k\), which in turn follows the validation loss development. This third building block is implemented between Step 19 and Step 21, where \(q_k\) is the current number of stored curvature pairs and \(m_{reset}\) is the memory size below which resetting is applied.

### 4. EXPERIMENTS

#### 4.1 Experimental Setup

In this section two implementations based on Algorithm 1 are considered: multi-batch L-BFGS with adaptive memory and without resetting (MB-AMR), i.e. \(m_{reset} = 0\), and multi-batch L-BFGS with both adaptive memory and resetting (MB-AMR), i.e. \(m_{reset} > 0\). In addition, a multi-batch L-BFGS with constant memory and periodic resetting, as proposed in McLoone and Irwin (1999), is considered. This variant, denoted as MB-R, performs resetting whenever the maximum memory size is reached. For benchmarking purposes, two additional methods are considered, namely, standard multi-batch L-BFGS (MB), and Adam. Therefore in total five methods are compared.

The six datasets and six experiments considered are detailed in Table 1 and Table 2, respectively. The MLP is a single-hidden layer fully connected feedforward neural network with \(h\) neurons in the hidden layer. The CNN has two 2D convolutional layers followed by two fully connected layers. Each convolutional layer is followed by a ReLU and a 2D max pooling layer. The function \(C(\cdot)\) in (1) minimized during training is the cross-entropy loss function (Bishop (2006)), with \(c(\cdot)\) defined as

\[
c(i), j(i) = -\{l(i) \ln(l(i)) + (1 - l(i)) \ln(1 - l(i))\}.
\]

The algorithms were written in PyTorch. The data augmentation of the TRASH dataset was performed using Keras. The experiments with the CNN were executed on an nVidia P40-4Q virtual GPU, while the experiments with the MLP were executed on a local desktop with an Intel i7-6700 CPU and 16 GB of RAM. The code is available on GitHub\(^2\).

Two metrics are used to assess algorithm performance: the correct classification rate (CCR) and the rank (RNK). CCR is defined as

\[
\text{CCR} = \frac{100}{|\mathcal{T}|} \sum_{i \in \mathcal{T}} z(i), \quad z(i) = \begin{cases} 1, & \text{if } l(i) = \hat{l}(i) \\ 0, & \text{otherwise} \end{cases}
\]

where \(\mathcal{T}\) is the test set. To evaluate RNK, for each simulation (60 in our experiments) we rank the five candidate

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1. https://github.com/hjmshi/PyTorch-LBFGS
2. https://github.com/fedsrcoco/AdaMultiLBFGS-PyTorch
3. Downloaded from: https://scikit-learn.org/stable/datasets/
4. Downloaded from: https://www.cs.ucl.ac.uk/~hvmom/datasets/
5. MNIST-R is a rescaled version of MNIST, which has 28 × 28 × 1 features.
6. Downloaded from: https://keras.io/datasets/
7. TRASH-RA is a rescaled and augmented version of TRASH, which has 512 × 384 × 3 features and 256T images in total.
8. Downloaded from: https://github.com/garythung/trashnet
9. Kernel size = 5 × 5, kernels per layer = 1, stride = 1, dilatation = 1, padding = 0, pool size = 2 × 2, pool stride = 2.
The mean and standard deviation of the final test CCR and RNK over these simulations, where “final” means the value once the training is completed. The last row of the table gives the mean and standard deviation over all six experiments, summarising the overall performance of each training algorithm.

The results vary considerably across the six experiments, with no single algorithm dominating. Adam achieves the best mean CCR performance in experiments 1, 3 and 6, MB-AM in experiments 4 and 5, and MB in experiment 2. Overall, MB-AM, MB-AMR and Adam yield similar mean CCR performance (74.1%–74.7%), with Adam having much lower variance in performance across the Monte Carlo simulations than the L-BFGS methods. MB-R is prone to converging to inferior solutions than the adaptive memory L-BFGS implementations and is reflected in the higher standard deviation in CCR (17.7% versus 11.9% for MB-AM, for example).

In terms of the rank metric, RNK, which considers the relative performance of each algorithm and is therefore less susceptible to outliers than CCR, MB-AM is the most consistently performing algorithm with a mean rank of 2.55, followed by MB-AMR with a mean rank of 2.58. MB is third at 2.8 and Adam is fourth at 3.2.

Table 4 shows the mean training computation time and, in parentheses, the mean time per iteration of the L-BFGS algorithms over the 60 Monte Carlo simulations normalized by the corresponding mean times for Adam. The algorithms have similar computation times for the three smaller dimension (MLP based) experiments, whereas MB-AM and MB-AMR are marginally faster than MB.
Fig. 2. The evolution of the training and test dataset cross-entropy loss and the test dataset CCR for a single simulation of each of the six experiments considered in the study.

Table 3. Mean (standard deviation) of CCR and RNK over 60 Monte Carlo simulations. The best results for each experiment are highlighted in bold.

| Experiment | MB | MB-AM | MB-R | MB-AMR | Adam |
|------------|----|-------|------|--------|------|
| MB         | CCR | RNK  | CCR  | RNK    | CCR  | RNK  |
| Exp. 1     | 80.9(15.8) | 3.3(1.48) | 85.0(13.8) | 2.5(1.44) | 84.7(13.4) | 3.0(1.36) | 85.8(12.3) | 2.6(1.32) | **90.1(1.4)** | **1.9(1.23)** |
| Exp. 2     | **65.0(21.3)** | **2.3(1.45)** | 61.5(15.5) | 2.6(1.14) | 59.6(15.7) | 2.4(1.17) | 58.2(19.8) | 2.7(1.31) | 53.5(0.0) | 4.1(0.87) |
| Exp. 3     | 87.5(16.6) | 3.8(1.22) | 91.5(19.9) | 2.7(1.36) | 95.9(9.8) | 2.9(1.40) | 95.0(12.3) | **2.2(1.43)** | **97.8(1.1)** | 3.3(1.03) |
| Exp. 4     | 87.6(36.1) | **1.8(1.24)** | **92.4(15.4)** | **2.8(1.14)** | 85.0(38.2) | 2.7(1.33) | 92.1(15.2) | 3.1(1.35) | 91.6(0.9) | 4.0(0.72) |
| Exp. 5     | 57.3(8.2) | 1.0(1.10) | **59.5(1.8)** | 2.0(0.85) | 48.9(8.3) | 4.0(0.52) | **57.8(8.8)** | **2.3(1.04)** | 53.1(1.2) | 4.1(0.84) |
| Exp. 6     | 49.6(12.2) | 3.4(1.03) | 55.7(5.6) | 2.7(0.89) | 39.9(5.0) | 4.9(0.37) | 55.5(6.4) | 2.6(0.89) | **62.4(1.6)** | **1.3(0.70)** |
| Mean       | 71.4(17.7) | 2.8(1.25) | 74.3(11.9) | **2.6(1.14)** | 69.0(13.6) | 3.4(1.01) | 74.1(12.2) | **2.6(1.17)** | **74.7(1.0)** | 3.2(0.87) |
when training the larger CNN based problems (3%-4%). This is a consequence of the low memory usage in early iterations which speeds up the L-BFGS two-loop recursion computation. The use of large batches and the computation of the approximated second order information make the L-BFGS methods substantially more computationally intensive than Adam and the advantage of the latter increases for the larger experiments. For example, Adam is more than 22 times faster than the L-BFGS algorithms for the MNIST case study (Experiment 4).

5. CONCLUSIONS

This paper has proposed three variants of the multi-batch L-BFGS algorithm of Berahas et al. (2016) based on the idea of progressive use of curvature information through a dev-increase scheme, and periodic memory resetting as introduced in McLoone and Irwin (1999). The experimental results show that the dev-increase adaptive memory scheme improves the generalisation performance and consistency of results obtained with L-BFGS and also slightly reduces its computational complexity. Periodic memory resetting is shown to be detrimental to performance, with MB-AMR marginally inferior to MB-AM and MB-R substantially inferior to MB. The overall ordering of algorithms in terms of generalisation performance is MB-AM, MB-AMR, MB, Adam and MB-R. In contrast, in terms of computational efficiency the order is Adam, MB-AM, MB-AMR, MB, and with Adam vastly superior to the other training algorithms. Therefore, Adam remains the algorithm of choice for training large neural networks, and only when the resulting accuracy is not satisfactory, should the use of MB-AM be considered.

MB-AM has the drawback of requiring three additional hyperparameters compared to MB (\( \alpha, m_0/m_{\text{max}} \) and \( m_{\text{val}} \)). The values used in this study are empirically defined and appropriate for a first investigation of the method. Future research will look at the automated selection of these parameters, and the potential for integrating MB-AM with progressive batching (Bollapragada et al. (2018)).

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