Large Scale Distributed Hessian-Free Optimization for Deep Neural Network

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Abstract
Training deep neural network is a high dimensional and a highly non-convex optimization problem. Stochastic gradient descent (SGD) algorithm and it’s variations are the current state-of-the-art solvers for this task. However, due to non-covexity nature of the problem, it was observed that SGD slows down near saddle point. Recent empirical work claim that by detecting and escaping saddle point efficiently, it’s more likely to improve training performance. With this objective, we revisit Hessian-free optimization method for deep networks. We also develop its distributed variant and demonstrate superior scaling potential to SGD, which allows more efficiently utilizing larger computing resources thus enabling large models and faster time to obtain desired solution. Furthermore, unlike truncated Newton method (Marten’s HF) that ignores negative curvature information by using naïve conjugate gradient method and Gauss-Newton Hessian approximation information - we propose a novel algorithm to explore negative curvature direction by solving the sub-problem with stabilized bi-conjugate method involving possible indefinite stochastic Hessian information. We show that these techniques accelerate the training process for both the standard MNIST dataset and also the TIMIT speech recognition problem, demonstrating robust performance with upto an order of magnitude larger batch sizes. This increased scaling potential is illustrated with near linear speed-up on upto 16 CPU nodes for a simple 4-layer network.

1 Introduction
Deep learning has shown great success in many practical applications, such as image classification [12, 23, 9], speech recognition [10, 22, 1], etc. Stochastic gradient descent (SGD), as one of the most well-developed method for training neural network, has been widely used. Besides, there has been plenty of interests in second-order methods for training deep networks [13]. The reasons behind these interests are multi-fold. At first, it is generally more substantial to apply weight updates derived from second-order methods in terms of optimization aspect, meanwhile, it takes roughly the same time to obtain curvature-vector products [11] as it takes to compute gradient which make it possible to use second-order method on large scale model. Furthermore, computing gradient and curvature information on large batch (even whole dataset) can be easily distributed across several nodes. Recent work has also been used to reveal the significance of identifying and escaping saddle point by second-order method, which helps prevent the dramatical deceleration of training speed around the saddle point [5].

Line search Newton-CG method (also known as the truncated Newton Method), as one of the practical techniques to achieve second-order method on high dimensional optimization, has been studied for decades [18]. Recent work to apply
Newton-CG method has been proved as a practical and successful achievement on training deep neural network\cite{13,11}. Indeed, for Newton-CG method, at each iteration, an approximated Hessian matrix is constructed, and naïve conjugate gradient (CG) method is applied to obtain a descent direction. The naïve CG method is, however, designed to solve positive definite systems, i.e., it requires the approximate Hessian matrix to be positive definite. Otherwise, the CG iteration is terminated as soon as a negative curvature direction is generated. Note that Newton-CG method does not require explicit knowledge of Hessian matrix, and it requires only the Hessian-vector product for any given vector. One special case for using Hessian-vector product is to train deep neural network, also known as Hessian-free optimization, and such Hessian-free optimization is exactly used in Marten’s HF\cite{13} methods.

As it is discussed in\cite{5}, to propose a way to identify and escape saddle point will significantly improve training performance. It implies the necessity to use negative curvature direction. While in Newton-CG methods, negative curvature direction is simply ignored, which may lead to limited performance of training. Small demo example is shown in this paper to highlight the importance of the using of negative curvature direction. In this paper, we derive ways to find negative curvature direction and propose new algorithm to use such negative curvature.

Moreover, it is well known that traditional SGD method, which is inherently sequential, is impractical to apply on very large data sets. More detail discussion can be found in\cite{28}, where Momentum SGD (MSGD)\cite{24}, ASGD and MVASGD\cite{20}, is considered. It is shown that these methods have limit scaling ability. However, unlike SGD, Hessian-free method can be distributed naturally and is able to improve convergence rate by increasing the mini-batch size, and we are therefore motivated to develop a distributed variant of Hessian-free optimization.

In this paper, we explore the Hessian-free methods to develop more robust and scalable solver for deep learning. We discuss novel ways to utilize negative curvature information to accelerate training speed. This is different with original Marten’s HF, where the negative curvature is ignored by either using Gauss-newton Hessian approximation or truncated Newton method. We perform experimental evaluations on two datasets without distortions or pre-training: hand written digits recognition (MNIST) and speech recognition (TIMIT).

Additionally, we explore hessian-free methods in a distributed context. Its potential scaling property is discussed, showcasing scaling potential of distributed Hessian-free method and how it allows taking advantage of more computing resources without being limited by the expensive communication.

2 Related Work

In recent years, in order to address the growing large scale machine learning problems, a plenty of researchers have explored/tried to scale-up machine learning algorithms through parallelization and distribution\cite{6,4}. Marten\cite{13} proposed the first framework to train deep network by second order method (HF). One more detailed work on HF is introduced in\cite{14}. Some other work with second order method include\cite{3} where a Jacobi preconditioned HF-CG solver was used,\cite{26} where a Krylov subspace descent (KSD) method to train deep network was analyzed and\cite{27} where HF for Cross-entropy training of a deep network was investigated. Note that KSD needs extra memory space to store a basis for Krylov subspace. L-BFGS method is proposed in\cite{17} and more practical techniques can be found in\cite{2}. With respect to SGD method, which is inherently sequential, it is impractical to implement it in a parallel environment. A variant of asynchronous stochastic gradient descent called Downpour SGD\cite{6} was hence designed. However, such ASGD does not scale well\cite{22}. Comparison results of the theoretical efficiency of model-parallel and data-parallel distributed stochastic gradient training for DNNs was shown and discussed in\cite{22}.

Negative curvature direction and its application in non-convex optimization has been studied for years\cite{19,7,15}. One can combine Newton type direction with (sufficient) negative curvature direction and proper line search to guarantee a convergence to a second order stationary point, e.g. a local minimum. Recent paper\cite{5} emphasized the importance on identifying and escaping saddle point to achieve better training performance, and saddle-free Newton (SFN) method was also proposed to handle negative curvature around the saddle point for small-size network.

Contributions.

- In this paper, we propose an algorithm which outperforms Newton-CG method is proposed. This is achieved by considering negative curvature information. The algorithm is able to escape saddle points in a cheaper way and therefore have better training performance.
- We evaluate the distributed variant of this second-order methods, showcasing its superior scaling property compared to conventional SGD. Unlike SGD method, which is inherently sequential and parallelism is limited to the small minibatches, which makes it the primary bottleneck to scaling and limits its usage on very large data sets. Our
second-order method inherently offers several orders of magnitude more parallelism and renders itself naturally to a distributed setting.

- We compare and analyze different methods both from algorithmic (convergence) and compute perspectives. We show in this paper that by using distributed Hessian-free method, we are able to achieve much better and stable scaling performance in terms of nodes and size of mini-batch.

## 3 Deep Neural Network in Distributed Environment

There are two natural ways how the problem of training DNN can be performed in parallel. The first one is known as mini-batch. In distributed HF, we only need synchronize once for gradient computing and other several times (much synchronizations/communications per epoch). In terms of SGD, where we need synchronize after every update which involving one gradient. As we will show in following sections, distributed HF need less synchronizations.

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Limits of SGD. As it can be seen from the estimates for amount of communication or the frequency of communication, choosing large value of $b$ will minimize communication and for data parallelism also amount of data sent. However, as it was observed e.g. in SGD (even for convex problem) can benefit from mini-batch only for small batch size $b$. After increasing $b$ above a critical value $b^*$, number of iterations needed to achieve a desired accuracy will not be decreased much if batch size $b > b^*$. Quite naturally this can be observed also for training DNN [4][28].

Benefits of Distributed HF. As we will show in following sections, distributed HF need less synchronizations/communications per epoch. In terms of SGD, where we need synchronize after every update which involving one mini-batch. In distributed HF, we only need synchronize once for gradient computing and other several times (much...
less than what we need of SGD, considering its limitation of using mini-batch size) which is related to number of CG iterations.

4 Distributed Hessian-free Optimization Algorithms

In this Section we describe a distributed Hessian-free algorithms. We assume that the size of the model is not huge and hence we choose data parallelism paradigm. We assume that the samples are split equally across $K$ computing nodes (MPI processes).

4.1 Distributed HF optimization framework

Within this Hessian-free optimization approach, for the sake of completeness, we first state the general Hessian-free optimization method \[13\] in Algorithm 1. Here $\theta \in \mathbb{R}^N$ is the parameters of this neural network. At $k$-th iteration, full

\begin{algorithm}
\caption{The Hessian-free optimization method}
\begin{algorithmic}
\State \textbf{for} $k = 1, 2, \ldots$ \textbf{do}
\State $g_k = \nabla f(\theta_k)$
\State Compute/adjust damping parameter $\lambda$
\State Define $B_k(d) = H(\theta_k)d + \lambda d$
\State $\tilde{p}_k = \text{CG-Minimize}(B_k, -g_k)$
\State $\theta_{k+1} = \theta_k + \tilde{p}_k$
\State \textbf{end for}
\end{algorithmic}
\end{algorithm}

gradient of error function $f(\theta_k)$ is evaluated and (approximated) Hessian matrix is defined as $H(\theta_k)$. Bases on this (approximated) Hessian and a proper damping parameter, which aims to make the damped Hessian matrix $B_k$ positive definite and/or avoid $B_k$ being singular. Afterwards, a quadratic approximation of $f$ around $\theta_k$ is constructed as

$$m_k(d) := f(\theta_k) + g_k^T d + \frac{1}{2} d^T B_k d.$$  \hfill (1)

If $B_k$ is positive definite, then we can obtain Newton step $d_k$ by letting $d_k := \text{arg min}_d m(d) = -B_k^{-1} g_k$. Otherwise, we solve $\min_d m(d)$ by CG method and choose the current iteration whenever a negative curvature direction is encountered, i.e., exist a vector $p$, such that $p^T B_k p < 0$. If the negative curvature direction is detected at the very first CG iteration, the steepest descent direction $-g_k$ is selected as a descent direction.

Marten \[13\] modified Algorithm 1 in several ways to make it suitable for DNNs. Within neural network, Hessian-vector can be calculated by a forward-backward pass which is roughly twice the cost of a gradient evaluation. On the other side, due to non-convexity of error function $f$, Hessian matrix is more likely to be indefinite and therefore a Gauss-Newton approximated Hessian-matrix is used. Note that Gauss-Newton is positive semidefinite matrix but it can be treated as a good approximation only if the current point is close to local minimizer, which motivates our work to design a Hybrid approach. Moreover, pre-conditioning and a CG-backtracking technique is used to decrease the number of CG iterations and obtain best descent direction. However, it is claimed in \[27\] that such techniques is not much helpful even make the performance worse since much more computation and storage space is needed. Therefore, we omit the two steps and further move to our distributed HF algorithm depicted in Algorithm 2. For example, to calculate full gradient (or Hessian vector product needed by CG solver), each node is responsible for computing the gradient (Hessian vector product) based on data samples stored locally. A reduction step is followed to aggregate them to a root node.

4.2 Dealing with Negative Curvature

As mentioned in \[5\], to minimize a non-convex error functions over continuous, high dimensional spaces, one may encounter proliferation of saddle points which are surrounded by high error plateaus. One shortage coming from the use of first-order methods like SGD is that it can not recognize curvature information, and therefore dramatically slow down the learning rate around such saddle points. The saddle-free Newton method (SFN) \[5\] is then proposed to identify and escape such saddle points. However, they build an exact Hessian to accomplish SFN on a small size neural network. However, this is impractical or even infeasible for medium or large scaled problems. In this paper, we propose another method to exploit the local non-convexity of the error function even for a large size network.
We are now ready to show an improved method to find a possible negative curvature by stabilized bi-conjugate gradient (Bi-CG-STAB) method. We show a 2D example [16] in Figure 2, where the function is $f(x, y) = 0.5x^2 + 0.25y^2 - 0.5xy^2$. It is easy to obtain that

$$\nabla f = (x, y^2 - y)^T,$$

and therefore three stationary points are obtained. Starting with any initial point of the form $(x, 0)^T$, the (stochastic) gradient descent method will always converge to saddle point $(0, 0)^T$. Actually, even for common second order method (Naive Newton method [18]), Saddle Free Newton method [13], they all converge to saddle point $(0, 0)^T$. The reason is that none of such algorithms can provide a direction along $y$-axis, which is a negative curvature direction. In this 2D-example, negative curvature direction can be chosen as $d = (0, -1)^T$ (the eigenvector associated to negative eigenvalue $-1$ of $\nabla^2 f$) at saddle point $(0, 0)^T$ and therefore, we escape saddle point $(0, 0)^T$ and achieve local minimum.

We are now ready to show an improved method to find a possible negative curvature by stabilized bi-conjugate gradient (Bi-CG-STAB) method [15], which is a Krylov method that can be used to solve unsymmetrical or indefinite linear system [21]. The benefits of using Bi-CG-STAB is that we can use exact stochastic Hessian information (which may not be positive definite) instead of using Gauss-newton approximation, which will lose the curvature information. It is shown in [13] that HF-CG is unstable and usually fails to convergence. The reason behind that is a fact that HF-CG ignores negative curvature. At the point where the Hessian has relative large amount of negative eigenvalues, it is also inefficient to find a descent direction by restarting the CG solver and modifying the damping parameter.

**Algorithm 2** Distributed Hessian-Free Algorithm

1: **Initialization:** $\theta_0$ (initial weights), $\lambda$ (initial damping parameter), $\delta_0$ (starting point for CG solver), $N$ (number of MPI processes), distributed data
2: for $k = 1, 2, \ldots$ do
3: Calculate gradient $\nabla f_{ij}(\theta_k)$ on each node $i = 0, \ldots, N - 1$
4: Reduce $\nabla f_{ij}(\theta_k)$ to root node to obtain full gradient $g_k = \frac{1}{N} \sum_{i=0}^{N-1} \nabla f_{ij}(\theta_k)$
5: Construct stochastic (approximated) Hessian-vector product operator $G_k(v)$
   - Calculate Hessian-vector product $\nabla^2 f_{ij}(\theta_k)v$ corresponding to one Mini-batch on each node $i = 0, \ldots, N - 1$
   - Reduce $\nabla^2 f_{ij}(\theta_k)v$ to root node to obtain $G_k(v) = \frac{1}{N} \sum_{i=0}^{N-1} \nabla^2 f_{ij}(\theta_k)v$
6: Solve $(G_k + \lambda I)(v) = -g_k$ by CG(BI-CG) method with starting point 0 or $\eta \delta_{k-1}$ ($\lambda$ is damping and $\eta$ is decay)
7: Use CG solution $s_k$ or possible negative curvature direction $d_k$ to find the best descent direction $\delta_k$
8: Update $\lambda$ by Levenberg-Marquardt method (Marten 2010)
9: Find $\alpha_k$ satisfying $f(\theta_k + \alpha_k \delta_k) \leq f(\theta_k) + \alpha_k g_k^T \delta_k$ (c is a parameter)
10: Update $\theta_{k+1} = \theta_k + \alpha_k \delta_k$
11: end for

A negative curvature direction at current point $\theta$ of function $f$ is defined as a vector such that the direction is descent ($g^T d \leq 0$) and also is dominant in the negative eigenspace ($d^T H d < 0$), where $g, H$ are gradient and Hessian of $f$ at point $\theta$.

One naive way how to find a negative curvature direction is to choose an eigenvector $u$ associated with a negative eigenvalue of $H$. Then a possible curvature direction is chosen from $\{-u, +u\}$ to ensure that $g^T d \leq 0$. Note that if positive semi-definite, no negative curvature direction can be found. In general, it is computationally expensive to find an eigenvector associated with smallest eigenvalue. Therefore a parameter $\mu \in (0, 1)$ is chosen and a sufficient negative descent direction should satisfy $d^T H d \leq \min(0, \mu \lambda_{\min}(H))$, where $\lambda_{\min}(H)$ is the smallest eigenvalue of $H$.

In other words, we intend to find negative curvature directions, i.e., direction $d$ such that $d^T H d < 0$. Actually, along with those negative directions, the approximated quadratic model is unbounded below, which shows potential of reduction at such direction (at least locally, while the quadratic approximation is valid). It was shown in [19] that if algorithms uses negative curvature directions, it will eventually converge to second-order critical point.

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We train MNIST and TIMIT dataset with various number of hidden layers and hidden units. Note that we do not do any distortions or pretraining for these two dataset as we are interested in scaling and stability of the methods.

5 Numerical Experiments

We study the multi-node scalability on the Endeavor cluster. Each Endeavor compute node has two Intel\textsuperscript{®} Xeon\textsuperscript{™} E5-2697v4 processors (18x2 cores), at a clock speed of 2.3 GHz and 128 GB DDR4 memory. The architecture features a super-scalar out-of-order micro-architecture supporting 2-way hyper-threading, resulting in the total of 72 hardware threads. In addition to scalar units, it has 8-wide single-precision SIMD units that support a wide range of SIMD instructions through Advanced Vector Extensions (AVX2)\textsuperscript{[8]}. In a single cycle, they can issue a 8-wide single-precision floating-point multiply and add, to two different pipelines. This allows for achieving full hardware utilization even when multiply and add can not be fused. Each core is backed by a 32 KB L1 and a 256 KB L2 cache, and all cores share an 45 MB last level L3 cache. Together, the 36 cores can deliver a peak performance of 2.65 Teraflops of single-precision arithmetic using AVX2. These compute nodes are connected with the HPC optimized Intel Omni-path (OPA) series 100 fabric with fat-tree topology. We use Intel MPI 5.1.3.181, and Intel compiler ICC 16.0.2.

We train MNIST and TIMIT dataset with various number of hidden layers and hidden units. Note that we do not do any distortions or pretraining for these two dataset as we are interested in scaling and stability of the methods.

Comparison of Distributed SGD and Distributed Hessian-free Variants. In Figure\textbf{3}, we train MNIST dataset with one hidden layers of 400 units, with $N = 16$ MPI processes and compare the performance of four algorithms in terms of the objective value vs. iterations (left), effective passes over data – epochs (middle) and number of communications (right). Note that for presentation purposes we count one epoch of SGD as "one iteration", even-thought it is $n/(N \times b)$ iterations. If we look on the evolution of objective value vs. iterations, all algorithms looks very comparable, however, if we check the evolution of objective value vs. epochs, we see that each iteration of second order method requires multiple epochs (one epoch for computing full gradient and possibly many more for a line-search procedure). We would

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{performance.png}
\caption{Performance comparison among SGD and Hessian-free variants.}
\end{figure}

Algorithm 3 Bi-CG-STAB Algorithm

1: Compute $r_0 := b - Ax_0$. Choose $r_0' := r_0$ such that $(r_0, r_0') \neq 0$
2: $p_0 := r_0$, $k := 0$
3: if Termination condition not satisfied then
4: $\alpha_j := (r_j, r_j')/(Ap_j, r_j')$
5: $s_j := r_j - \alpha_j Ap_j$
6: $\gamma_j := (s_j, As_j)/(As_j, As_j)$
7: $x_{j+1} := x_j + \alpha_j p_j + \gamma_j s_j$
8: $r_{j+1} := s_j - \gamma_j As_j$
9: $\beta_j := (r_{j+1}, r_{j+1}')/(r_j, r_0')^2 \times \frac{\alpha_j}{\gamma_j}$
10: $p_{j+1} := r_{j+1} + \beta_j (p_j - \gamma_j A p_j)$
11: end if

\[1\text{Intel, Xeon, and Intel Xeon Phi are trademarks of Intel Corporation in the U.S. and/or other countries. Software and workloads used in performance tests may have been optimized for performance only on Intel microprocessors. Performance tests, such as SYSmark and MobileMark, are measured using specific computer systems, components, software, operations and functions. Any change to any of those factors may cause the results to vary. You should consult other information and performance tests to assist you in fully evaluating your contemplated purchases, including the performance of that product when combined with other products. For more information go to http://www.intel.com/performance}
Scaling Properties of Distributed Hessian-free Methods. Let us now study scaling properties of existing and proposed distributed Hessian-free methods. All experiments in this section were done on TIMIT speech recognition dataset, with 360 features, 1973 classes, and 101350 samples. The samples are split into two parts, where we use 70% as training dataset and 30% as testing dataset. The network is set to have 3 fully-connected hidden layers with 512 units each. In Figure 5 (top-left) we show the scaling or all studied second order methods with respect to the number of nodes. Each node has two sockets, which correspond to two non-uniform memory NUMA regions. To exploit this we run a MPI rank per socket and within the socket we use the multi-threaded MKL implementation of the BLAS function (sgemm, sgemv) to utilize the 18 cores.

The picture on left shows how the duration of one iteration scale with number of nodes for various size of batch size. Observe, that the scaling is almost linear for values $B \geq 4096$. Actually, the small batch size is the primary bottleneck for scaling because of the limited parallelism. Hence a larger batchsize (increased parallelism) is essential for scaling to larger number of nodes. As was show in [4] large batchsize are generally only beneficial for second order methods (as opposed to SGD). Figure 6 (top, last 3 plots) shows the speed-up property of the 3 main components of the second order algorithm. Note that both gradient computation and line search inherit similar behaviour as the total cost of one iteration. In case of CG, we see that the time of one CG is increasing with increasing size of nodes. The reason for it is that Hessian-vector product is evaluated only for one batch (whose time should be independent from the number of nodes used) but the communication time is naturally increased with mode nodes. It reminds us to remark that the time of communication in this case is comparable to the local compute and hence the pictures suggest very bad scaling. Let us stress that the time of one CG is in order of magnitude smaller then computing of full gradient or line search procedure. As an immediate next step, we are looking into more comprehensive characterization of the compute and

Figure 4: Performance comparison among various size of mini-batches on different methods (left 3 plots), and number of iterations required to obtain training error 0.02 as a function of batch size for second order methods. The neural network has two hidden layers with size 400, 150.
bottleneck analysis of both single and multinode performance. Figure 5 (bottom) shows the each batch size the time of 3 major components of the algoritm.

6 Conclusion

In this paper, we revisited HF optimization for deep neural network, proposed a distributed variant with analysis. We showed that unlike the parallelism of SGD, which is inherently sequential, and has limitation (large batch-size helps to scale it but slows convergence). Moreover, a cheap way to detect curvature information and use negative curvature direction by using BI-CG-STAB method is discussed. It is known that to use of negative curvature direction is essential on improves the training performance. Furthermore, a Hybrid variant is discussed and applied. We show a significant speed-up by applying distributed HF in numerical experiment and the basic comparison among SGD and other HF method shows a competitive performance.

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Appendix

In this Section we show evolution of training error and objective value for various number of hidden layers. This again shows, that the BI-CG-STAB is able to utilize negative curvature and hence outperforms other second order variants studied in this paper.