Practical Quasi-Newton Methods for Training Deep Neural Networks

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Abstract

We consider the development of practical stochastic quasi-Newton, and in particular Kronecker-factored block-diagonal BFGS and L-BFGS methods, for training deep neural networks (DNNs). In DNN training, the number of variables and components of the gradient is often of the order of tens of millions and the Hessian has $n^2$ elements. Consequently, computing and storing a full $n \times n$ BFGS approximation or storing a modest number of (step, change in gradient) vector pairs for use in an L-BFGS implementation is out of the question. In our proposed methods, we approximate the Hessian by a block-diagonal matrix and use the structure of the gradient and Hessian to further approximate these blocks, each of which corresponds to a layer, as the Kronecker product of two much smaller matrices. This is analogous to the approach in KFAC [29], which computes a Kronecker-factored block-diagonal approximation to the Fisher matrix in a stochastic natural gradient method. Because the indefinite and highly variable nature of the Hessian in a DNN, we also propose a new damping approach to keep the upper as well as the lower bounds of the BFGS and L-BFGS approximations bounded. In tests on autoencoder feed-forward neural network models with either nine or thirteen layers applied to three datasets, our methods outperformed or performed comparably to KFAC and state-of-the-art first-order stochastic methods.

1 Introduction

We consider in this paper the development of practical stochastic quasi-Newton (QN), and in particular Kronecker-factored block-diagonal BFGS [6, 13, 16, 37] and L-BFGS [26], methods for training deep neural networks (DNNs). Recall that the BFGS method starts each iteration with a symmetric positive definite matrix $B$ (or $H = B^{-1}$) that approximates the current Hessian matrix (or its inverse), computes the gradient $\nabla f$ of $f$ at the current iterate $x$ and then takes a step $s = -\alpha H \nabla f$, where $\alpha$ is a step length (usually) determined by some inexact line-search procedure, such that $y^T s > 0$, where $y = \nabla f^+ - \nabla f$ and $\nabla f^+$ is the gradient of $f$ at the new point $x^+ = x + s$. The method then computes an updated approximation $B^+$ to $B$ (or $H^+ to H$) which remains symmetric and positive-definite and satisfies the so-called quasi-Newton (QN) condition $B^+ s = y$ (or equivalently, $H^+ y = s$). A consequence of this is that the matrix $B^+$ operates on the vector $s$ in exactly the same way as the average of the Hessian matrix along the line segment between $x$ and $x^+$ operates on $s$.

In DNN training, the number of variables and components of the gradient is often of the order of tens of millions and the Hessian has $n^2$ elements. Hence, computing and storing a full $n \times n$ BFGS approximation or storing $M (s, y)$ pairs, where $M$ is approximately 10 or larger for use in an L-BFGS implementation, is out of the question. Consequently, in our methods, we approximate the Hessian by a block-diagonal matrix, where each diagonal block corresponds to a layer, further approximating them as the Kronecker product of two much smaller matrices, as in [29, 5, 19, 10].

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Literature Review on Using Second-order Information for DNN. For solving the stochastic optimization problems with high-dimensional data that arise in machine learning, stochastic gradient descent (SGD) and its variants are the methods that are most often used, especially for training DNNs. These variants include such methods as AdaGrad [12], RMSprop [21], and Adam [24], all of which scale the stochastic gradient by a diagonal matrix based on estimates of the first and second moments of the individual gradient components. Nonetheless, there has been a lot of effort to find ways to take advantage of second-order information in solving ML optimization problems. Approaches have run the gamut from [4], use of a diagonal re-scaling of the stochastic gradient, based on the secant condition associated with quasi-Newton (QN) methods, to sub-sampled Newton methods (e.g., see [40], and references therein), including those that solve the Newton system using the linear conjugate gradient method (see [8]).

In between these two extremes are stochastic methods that are based either on QN methods or generalized Gauss-Newton (GGN) and natural gradient [1] methods. For example, a stochastic L-BFGS method for solving strongly convex problems was proposed by [9] that uses sampled Hessian-vector products rather than gradient differences, which [32] proved to be linearly convergent by incorporating the variance reduction technique (SVRG [23]) to alleviate the effect of noisy gradients. A closely related variance reduced block L-BFGS method was proposed by [17]. [30] proposed a regularized stochastic BFGS method, and an online L-BFGS method was proposed in [31] for strongly convex problems which was extended by [27] to incorporate SVRG variance reduction. Stochastic BFGS and L-BFGS methods were also developed for online convex optimization in [36]. For nonconvex problems, [39] developed a damped L-BFGS method which incorporated SVRG variance reduction and studied its convergence properties.

GGN methods that approximate the Hessian have been proposed, including the Hessian-free method [28] and the Krylov subspace method [38]. Variants of the closely related natural gradient method that use block-diagonal approximations to the Fisher information matrix, where blocks correspond to layers, have been proposed in e.g. [20, 11, 29, 14]. Using further approximation of each of these (empirical) Fisher matrix and GNN blocks by the Kronecker product of two much smaller matrices, [29], [5], [15], and [19] developed the efficient KFAC, KFRA, EKFAC, and Shampoo methods, respectively. See also [2] and [10], [35], which combines both Hessian and covariance (Fisher-like) matrix information in a stochastic Newton type method.

Our Contributions. The main contributions of this paper can be summarized as follows:
1. New BGFS and L-BFGS methods that take advantage of the structure of feed-forward DNN training problems;
2. Efficient non-diagonal second-order algorithms for deep learning that require a comparable amount of memory and computational cost per iteration as first-order methods;
3. A new damping scheme for BFGS and L-BFGS updating of an inverse Hessian approximation, that not only preserves its positive definiteness, but also limits the decrease (and increase) in its smallest (and largest) eigenvalues for non-convex problems;
4. A novel application of Hessian-action BFGS;
5. The first proof of convergence (to the best of our knowledge) of a stochastic Kronecker-factored quasi-Newton method.

2 Kronecker-factored Quasi-Newton Method for DNN

After reviewing the computations used in DNN training, we describe the Kronecker structures of the gradient and Hessian for a single data point, followed by their extension to approximate expectations of these quantities for multiple data-points and give a generic algorithm that employs BFGS (or L-BFGS) approximations for the Hessians.

Deep Neural Networks. We consider a feed-forward DNN with \( L \) layers, defined by weight matrices \( W_l \) (whose last columns are bias vectors \( b_l \)) and activation functions \( \phi_l \) for \( l \in \{1 \ldots L\} \) and loss function \( \mathcal{L} \). For an input data-point \((x, y)\), the loss \( \mathcal{L}(a_L, y) \) between the output \( a_L \) of the DNN and \( y \) is a non-convex function of \( \theta = \begin{bmatrix} \text{vec}(W_1)^\top, \ldots, \text{vec}(W_L)^\top \end{bmatrix}^\top \). The network’s forward and backward pass for a single input data point \((x, y)\) is described in Algorithm 1.
Algorithm 1 Forward and backward pass of DNN for a single data-point

1: given input \((x, y)\), weights (and biases) \(W_l\), and activations \(\phi_l\) for \(l \in [1, L]\)
2: \(a_0 = x; \) for \(l = 1, \ldots, L\) do \(a_{l-1} = (a_{l-1}, 1); h_l = W_l a_{l-1}; a_l = \phi_l(h_l)\)
3: \(D a_L \leftarrow \frac{\partial L(x,y)}{\partial z}|_{z=a_L}\)
4: for \(l = L, \ldots, 1\) do \(g_l = D a_l \odot \phi'_l(h_l); D W_l = g_l a_{l-1}^T; D a_{l-1} = W_l^T g_l\)

For a training dataset that contains multiple data-points indexed by \(i = 1, \ldots, I\), let \(f(i; \theta)\) denote the loss for the \(i\)th data-point. Then, viewing the dataset as an empirical distribution, the total loss function \(f(\theta)\) that we wish to minimize is

\[
f(\theta) := \mathbb{E}_i[f(i; \theta)] := \frac{1}{I} \sum_{i=1}^{I} f(i; \theta).
\]

Single Data-point: Layer-wise Structure of the Gradient and Hessian. Let \(\nabla f_i\) and \(\nabla^2 f_i\) denote, respectively, the restriction of \(\nabla f\) and \(\nabla^2 f\) to the weights \(W_l\) in layer \(l = 1, \ldots, L\). For a single data-point \(\nabla f_i\) and \(\nabla^2 f_i\) have a tensor (Kronecker) structure, as shown in [29] and [5]. Specifically,

\[
\nabla f_i(i) = g_i(i)(a_{l-1}(i))^T, \quad \text{equivalently,} \quad \text{vec}(\nabla f_i(i)) = a_{l-1}(i) \odot g_i(i), \tag{1}
\]

\[
\nabla^2 f_i(i) = (a_{l-1}(i)(a_{l-1}(i))^T) \otimes G_l(i), \tag{2}
\]

where the pre-activation gradient \(g_i(i) = \frac{\partial f_i(i)}{\partial h_l(i)}\), and the pre-activation Hessian \(G_l(i) = \frac{\partial^2 f_i(i)}{\partial h_l(i)^2}\). Our algorithm uses an approximation to \((G_l(i))^{-1}\), which is updated via the BFGS updating formulas based upon a secant condition that relates the change in \(g_i(i)\) with the change in \(h_l(i)\).

Multiple Data-points: Kronecker-factored QN Approach. Now consider the case where we have a dataset of \(I\) data-points indexed by \(i = 1, \ldots, I\). By (2), we have

\[
\mathbb{E}_i[\nabla^2 f_i(i)] \approx \mathbb{E}_i[(a_{l-1}(i)(a_{l-1}(i))^T)] \odot \mathbb{E}_i[G_l(i)] := A_l \otimes G_l \tag{3}
\]

Note that the approximation in (3) that the expectation of the Kronecker product of two matrices equals the Kronecker product of their expectations is the same as the one used by K-FAC [29]. Now, based on this structural approximation, we use \(H^l = H^l_a \otimes H^l_g\) as our QN approximation to \([\mathbb{E}_i[\nabla^2 f_i(i)]]^{-1}\), where \(H^l_a\) and \(H^l_g\) are positive definite approximations to \(A^{-1}_l\) and \(G_l^{-1}\), respectively. Hence, with the block-diagonal assumption on Hessian, a step in our algorithm is computed as

\[
\text{vec}(W_i^+) - \text{vec}(W_i) = -\alpha H^l \text{vec} \left( \nabla f_i \right) = -\alpha (H^l_a \otimes H^l_g) \text{vec} \left( \nabla f_i \right) = -\alpha \text{vec} \left( H^l_a \nabla f_i H^l_a^T \right), \tag{4}
\]

where \(\nabla f_i\) denotes the estimate to \(\mathbb{E}_i[\nabla f_i(i)]\) and \(\alpha\) is the learning rate. After computing \(W_i^+\) and performing another forward/backward pass, our method computes or updates \(H^l_a\) and \(H^l_g\) as follows:

1. For \(H^l_g\), we use a damped version of BFGS (or LBFGS) (See Section 3) based on the \((s, y)\) pairs corresponding to the average change in \(h_l(i)\) and the average change in the gradient with respect to \(h_l(i)\); i.e.,

\[
s_g^l = \mathbb{E}_i[h_i^+(i)] - \mathbb{E}_i[h_l(i)], \quad y_g^l = \mathbb{E}_i[g_i^+(i)] - \mathbb{E}_i[g_l(i)]. \tag{5}
\]

2. For \(H^l_a\) we use the "Hessian-action" BFGS method described in Section 4. The issue of possible singularity of the positive semi-definite matrix \(A_l\) approximated by \((H^l_a)^{-1}\) is also addressed there by incorporating an Levenberg-Marquardt (LM) damping term.

A high-level summary of the K-BFGS and K-BFGS(L) algorithms is given in Algorithm 2 (see Algorithm 4 in the appendix for a detailed pseudocode). We name our algorithms K-BFGS and K-BFGS(L) if we use BFGS or LBFGS to update \(H^l_g\), respectively. The use of mini-batches is described in Section 6.
Algorithm 2 High-level summary of K-BFGS / K-BFGS(L)

Require: Given initial weights $\theta$, batch size $m$, learning rate $\alpha$
1: for $k = 1, 2, \ldots$ do
2: Sample mini-batch of size $m$: $M_k = \{x_{k,i}, i = 1, \ldots, m\}$
3: Perform a forward-backward pass over the current mini-batch $M_k$ (see Algorithm 1)
4: for $l = 1, \ldots, L$ do $p_l = H^l_y \nabla f_l \nabla H^l_y$, $W_l = W_1 - \alpha \cdot p_l$
5: Perform another forward-backward pass over $M_k$ to get $(s^l_y, y^l_y)$
6: Use damped BFGS or LBFGS to update $H^l_y$ ($l = 1, \ldots, L$) (see Section 3, in particular Algorithm 3)
7: Use Hessian-action BFGS to update $H^l_a$ ($l = 1, \ldots, L$) (see Section 4)

3 BFGS and LBFGS for $G_l$

Damped BFGS Updating. It is well-known that training a DNN is a non-convex optimization problem. As (2) and (3) show, this non-convexity manifests in the fact that $G_l$ ≥ 0 often does not hold. Thus, in order to use BFGS updating for $H^l_y$, the approximation to $G_l^{-1}$, we have to handle the indefiniteness of $G_l$ to make sure that $(s^l_y)^T y^l_y > 0$. Due to the stochastic setting, ensuring this condition, which is sufficient for maintaining positive-definiteness of $H^l_y$, by line-search as is done in deterministic settings, is very expensive. In addition, due to the large changes in curvature in DNN models that occur as the parameters are varied, we also need to suppress large changes to $H^l_y$ as it is updated. To deal with both non-convexity and stochasticity, we propose a double damping (DD) procedure (Algorithm 3), which is based upon Powell’s damped-BFGS approach [34], for modifying the $(s^l_y, y^l_y)$ pair. To motivate Algorithm 3, consider the formulas used for BFGS updating of $B$ and $H$:

$$B^+ = B - \frac{Bss^T s}{s^T Bs} + \rho yy^T, \quad H^+ = (I - \rho yy^T)H(I - \rho yyy^T) + \rho yy^T,$$

where $\rho = \frac{1}{s^T y} > 0$. If we can ensure that $0 < \frac{y^T H y}{s^T y} \leq \frac{1}{\mu_3}$ and $0 < \frac{s^T s}{s^T y} \leq \frac{1}{\mu_2}$, then we can obtain the following bounds:

$$\|B^+\| \leq \|B - \frac{Bss^T s}{s^T Bs}\| + \|\rho yy^T\| \leq \|B\| + \|\frac{B^{1/2} H^{1/2} yy^T H^{1/2} B^{1/2}}{s^T y}\| \quad (7)$$

and

$$\|H^+\| \leq \|H^{1/2} - \frac{sy^T H^{1/2}}{s^T y}\|^2 + \|\frac{ss^T}{s^T y}\| \leq \left(\|H^{1/2}\| + \|\frac{ss^T}{s^T y}\|\right)^2 + \|\frac{s^T s}{s^T y}\|^2 \quad (9)$$

Thus, the change in $B$ (and $H$) is controlled if $\frac{y^T H y}{s^T y} \leq \frac{1}{\mu_3}$ and $\frac{s^T s}{s^T y} \leq \frac{1}{\mu_2}$. Our DD approach is a two-step procedure, where the first step (i.e. Powell’s damping on $H$) guarantees that $\frac{y^T H y}{s^T y} \leq \frac{1}{\mu_3}$ and the second step (i.e., Powell’s damping with $B = I$) guarantees that $\frac{s^T s}{s^T y} \leq \frac{1}{\mu_2}$. Note that there is no guarantee of $\frac{y^T H y}{s^T y} \leq \frac{1}{\mu_3}$ after the second step. However, we can skip updating $H$ in this case so that the bounds on these matrices hold. In our implementation, we always do the update, since in empirical testing, we observed that at least 90% of the pairs satisfy $\frac{y^T H y}{s^T y} \leq \frac{2}{\mu_3}$. See Section C in the appendix for more details on damping.

LBFGS Implementation. LBFGS can also be used to update $H^l_y$. However, implementing LBFGS using the standard “two-loop recursion” (see Algorithm 7.4 in [33]) is not efficient. This is because the main work in computing $H^l_y \nabla f_l H^l_y$ in line 4 of Algorithm 2 would require $4p$ matrix-vector
When QN update in the O whose main work involves 2 matrix-matrix multiplications, each requiring Algorithm 3 Double Damping (DD) term to make our "Hessian-action" BFGS stable; i.e., we use (LM) damping Theorem 1. Suppose that Levenberg-Marquardt Levenberg-Marquardt Damping for A by 1 simplifying, one obtains A tion formula to n linearly independent set of s H
Proof. If s y y H y then \( \theta_1 = \frac{1 - \mu_1 y^THy}{y^THy - s^T y} \) else \( \theta_1 = 1 \)
4 "Hessian action" BFGS for A
In addition to approximating \( G^{-1}_1 \) by \( H_0 \) using BFGS, we also propose approximating \( A^{-1} \) by \( H_0 \) using BFGS. Note that \( A \) does not correspond to some Hessian of the objective function. However, we can generate \((s, y)\) pairs for it by "Hessian action" (see e.g. [9, 17, 18]).

Connection between Hessian-action BFGS and Matrix Inversion. In our methods, we choose s = \( H_a \) and y = \( A^+ \) s, where \( A^+ = A + c \cdot a a^\top \); i.e., only a rank-one update is made to A. This corresponds to the case where the information of A is accumulated from iteration to iteration, and the size of the mini-batch is 1 or \( a \) represents the average of the vectors a(i) from multiple data-points.

Theorem 1. Suppose that A and H are symmetric and positive definite, and that H = A^{-1}. If we choose s = \( H_a \) and y = \( A^+ \) s, where \( A^+ = A + c \cdot a a^\top \) (c > 0). Then, the \( H^+ \) generated by any QN update in the Broyden family
\[
H^+ = H - \sigma H y y^\top H + \rho s s^\top + \phi(y^\top H y) h h^\top,
\]
where \( \rho = 1/s^\top y, \sigma = 1/y^\top H y, h = \rho s - \sigma H y \) and \( \phi \) is a scalar parameter in [0, 1], equals \((A^+)^{-1}\). Note that \( \phi = 1 \) yields the BFGS update (6) and \( \phi = 0 \) yields the DFP update.

Proof. If s = \( H_a \) and y = \( A^+ \) s, then h = 0, so all choices of \( \phi \) yield the same matrix \( H^+ \). Since \( H^+ A^+ s = H^+ y = s \) and for any vector v that is orthogonal to a, \( H^+ A^+ v = H^+ A v = v \), since \( s^\top A v = 0 \) and \( y^\top H A v = 0 \), it follows that \( H^+ A^+ = I \), using the fact that s together with any linearly independent set of \( n - 1 \) vectors orthogonal to a spans \( R^n \). (Note that \( s^\top a = a^\top H_a a \geq 0 \), since \( H \succeq 0 \) ⇒ that s is not orthogonal to a.)

In fact, all updates in the Broyden family are equivalent to applying the Sherman-Morrison modification formula to \( A^+ = A + c \cdot a a^\top \), given \( H = A^{-1} \), since after substituting for s and y in (11) and simplifying, one obtains
\[
H^+ = H - H a (c^{-1} + a^\top H a)^{-1} a^\top H.
\]
In the multiple data-points case, we choose s = \( H \cdot E_a[a(i)] \). When using momentum, \( A^+ = \beta A + (1 - \beta) a a^\top \) (0 < \( \beta < 1 \); hence, if we still want Theorem 1 to hold, we have to scale H by 1/\( \beta \) before updating it. This, however, turns out to be unstable. Hence, we choose to use the non-scaled version of "Hessian action" BFGS.

Levenberg-Marquardt Damping for A. Since \( A_t = E_t \left[ (a_{t-1}(i) a_{t-1}(i))^\top \right] \geq 0 \) may not be positive definite, or may have very small positive eigenvalues, we add an Levenberg-Marquardt (LM) damping term to make our "Hessian-action" BFGS stable; i.e., we use \( A_t + \lambda A \) instead of \( A_t \), when we update \( H_a \). Specifically, "Hessian action" BFGS for \( A_t \) is performed as
1. \( A_t = \beta \cdot A_t + (1 - \beta) \cdot E_t \left[ a_{t-1}(i) a_{t-1}(i)^\top \right] ; A_t^{LM} = A_t + \lambda A \).
2. \( s_t^i = H_a \cdot E_t[a_{t-1}(i)], y_t^i = A_t^{LM} s_t^i, \) Use BFGS with \((s_t^i, y_t^i)\) to update \( H_a \).
5 Convergence Analysis

Following the framework for stochastic quasi-Newton methods (SQN) established in [39] for solving nonconvex stochastic optimization problems (see Section B in the appendix for the framework), we prove that, under fairly standard assumptions, for our K-BFGS(L) algorithm with skipping DD and exact inversion on $A_l$ (see Algorithm 5 in Section B), the number of iterations $N$ needed to obtain 
\[ \frac{1}{N} \sum_{k=1}^{N} \mathbb{E} \left[ \| \nabla f(\theta_k) \|^2 \right] \leq \epsilon \] is $N = O(\epsilon^{-\frac{1}{1-\beta}})$, for step size $\alpha_k$ chosen proportional to $k^{-\beta}$, where $\beta \in (0.5, 1)$ is a constant. Our proofs, which are delayed until Section B, make use of the following assumptions, the first two of which, were made in [39].

**AS. 1.** $f: \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable. $f(\theta) \geq f^{\text{low}} > -\infty$, for any $\theta \in \mathbb{R}^n$. $\nabla f$ is globally $L$-Lipschitz continuous; namely for any $x, y \in \mathbb{R}^n$, $\| \nabla f(x) - \nabla f(y) \| \leq L \| x - y \|$. 

**AS. 2.** For any iteration $k$, the stochastic gradient $\hat{\nabla f}_k = \hat{\nabla f}(\theta_k, \xi_k)$ satisfies: a) $\mathbb{E}_{\xi_k} \left[ \hat{\nabla f}(\theta_k, \xi_k) \right] = \nabla f(\theta_k)$, b) $\mathbb{E}_{\xi_k} \left[ \| \hat{\nabla f}(\theta_k, \xi_k) - \nabla f(\theta_k) \|^2 \right] \leq \sigma^2$, where $\sigma > 0$, and $\xi_k, k = 1, 2, \ldots$ are independent samples that are independent of $\{\theta_j\}_{j=1}^\infty$.

**AS. 3.** The activation functions $\phi_i$ have bounded values: $\exists \varphi > 0$ s.t. $\forall l, \forall h, |\phi_i(h)| \leq \varphi$.

To use the convergence analysis in [39], we need to show that the block-diagonal approximation of the inverse Hessian used in Algorithm 5 satisfies the assumption that it is bounded above and below by positive-definite matrices. Given the Kronecker structure of our Hessian inverse approximation, it suffices to prove boundness of both $H^1_k(k)$ and $H^2_k(k)$ for all iterations $k$. Making the additional assumption AS.3, we are able to prove Lemma 1, and hence Lemma 3, below. Note that many popular activation functions satisfy Assumption 3, such as sigmoid and tanh.

**Lemma 1.** Suppose that AS.3 holds. There exist two positive constants $\kappa_a, \bar{\kappa}_a$ such that $\kappa_a I \preceq H^1_k(k) \preceq \bar{\kappa}_a I, \forall k, l$.

**Lemma 2.** There exist two positive constants $\kappa_g$ and $\bar{\kappa}_g$, such that $\kappa_g I \preceq H^1_g(k) \preceq \bar{\kappa}_g I, \forall k, l$.

**Lemma 3.** Suppose that AS.3 holds. Let $\theta_{k+1} = \theta_k - \alpha_k H_k \hat{\nabla f}_k$ be the step taken in Algorithm 5. There exists two positive constants $\bar{\kappa}, \bar{\kappa}$ such that $\bar{\kappa} I \preceq H_k \preceq \bar{\kappa} I, \forall k, l$.

Using Lemma 3, we can now apply Theorem 2.8 in [39] to prove the convergence of Algorithm 5:

**Theorem 2.** Suppose that assumptions AS.1-3 hold for $\{\theta_k\}$ generated by Algorithm 5 with mini-batch size $m_k = m$ for all $k$, and $\alpha_k$ is chosen as $\alpha_k = \frac{\kappa}{L} k^{-\beta}$, with $\beta \in (0.5, 1)$. Then
\[ \frac{1}{N} \sum_{k=1}^{N} \mathbb{E} \left[ \| \nabla f(\theta_k) \|^2 \right] \leq \frac{2L (M_f - f^{\text{low}})}{\kappa^2} N^{1-\beta} + \frac{\sigma^2}{(1-\beta)m} \left( N^{-\beta} - N^{-1} \right) \]
where $N$ denotes the iteration number and $M_f > 0$ depends only on $f$. Moreover, for a given $\epsilon \in (0, 1)$, to guarantee that $\frac{1}{N} \sum_{k=1}^{N} \mathbb{E} \left[ \| \nabla f(\theta_k) \|^2 \right] < \epsilon$, the number of iterations $N$ needed is at most $O \left( \epsilon^{-\frac{1}{1-\beta}} \right)$.

Note: other theorems in [39], namely Theorems 2.5 and 2.6, also apply here under our assumptions.

6 Experiments

Before we present some experimental results, we address the use of moving averages, and the computational and storage requirements of the algorithms that we tested.

**Mini-batch and Moving Average.** Clearly, using the whole dataset at each iteration is inefficient; hence, we use a mini-batch to estimate desired quantities. We use $\hat{X}$ to denote the averaged value of $X$ across the mini-batch for any quantity $X$. To incorporate information from the past as well as reducing the variability, we use an exponentially decaying moving average to estimate desired quantities with decay parameter $\beta \in (0, 1)$:

1. To estimate the gradient $\mathbb{E}_i [\nabla f(i)]$, at each iteration, we update $\hat{\nabla f} = \beta \cdot \hat{\nabla f} + (1 - \beta) \cdot \nabla f$. 


2. $H_t$: To estimate $A_t$, at each iteration we update $\hat{A}_t = \beta \cdot \hat{A}_t + (1 - \beta) \cdot a_{t-1} a_{t-1}^\top$.
3. $H_t$: BFGS “uses” momentum implicitly incorporated in the matrices $H_t$. To further stabilize the BFGS update, we also use a moving-averaged $(s_t, y_t)$ (before damping); i.e., We update $s_t = \beta \cdot s_{t-1} + (1 - \beta) \cdot (\nabla f_t - \nabla f_{t-1})$, and $y_t = \beta \cdot y_{t-1} + (1 - \beta) \cdot (g_t - g_{t-1})$.

Finally, when computing $\overline{h_t}$ and $\overline{g_t}$, we use the same mini-batch as used to compute $\overline{h_t}$ and $\overline{g_t}$. This doubles the number of forward-backward passes at each iteration.

**Storage and Computation.** Tables 1 and 2 compare the storage and computational requirements, respectively, for a layer with $d_i$ inputs and $d_o$ outputs for K-BFGS, K-BFGS(L), KFAC, and Adam/RMSprop. We denote the size of mini-batch by $m$, the number of $(s, y)$ pairs stored for LBFGS by $p$, and the frequency of matrix inversion in KFAC by $T$. Besides the requirements listed in Table 1, all algorithms need storage for the parameters $W_i$ and the estimate of the gradient, $\nabla f_t$, (i.e. $O(d_i d_o)$). Besides the work listed in Table 2, they also need to do a forward-backward pass to compute $\nabla f_t$ as well as updating $W_i$, (i.e. $O(md_i d_o)$). Also note that, even though we use big-O notation in these tables, the constants for all of the terms in each of the rows are roughly at the same level and relatively small.

In Table 2, for K-BFGS and K-BFGS(L), "Additional pass” refers to Line 5 of Algorithm 2; under “Curvature”, $O(md_i^2)$ arises from “Hessian action” BFGS to update $H_a$ (see the algorithm in the end of Section 4); $O(md_o^2)$ arises from (5), $O(d_o^2)$ arises from updating $H_b^l$ (only for K-BFGS); and “Step $\Delta W_t$” refers to (4). For KFAC, referring to Algorithm 7 (in the appendix), “Additional pass” refers to Line 7; under "Curvature", $O(md_i^2 + md_o^2)$ refers to Line 8, and $O(\frac{1}{\tau}d_i^3 + \frac{1}{\tau}d_o^3)$ refers to Line 10; and "Step $\Delta W_t$" refers to Line 5.

From Table 1, we see that the Kronecker property enables K-BFGS and K-BFGS(L) (as well as KFAC) to have storage requirements comparable to those of first-order methods. Moreover, from Table 2, we see that K-BFGS and K-BFGS(L) require less computation per iteration than KFAC, since they only involve matrix multiplications, whereas KFAC requires matrix inversions which depend cubically on both $d_i$ and $d_o$. The cost of matrix inversion in KFAC (and singular value decomposition in [19]) is amortized by performing these operations only once every $T$ iterations; nonetheless, these amortized operations usually become much slower than matrix multiplication as models scale up.

### Table 1: Storage

| Algorithm     | $\nabla f_t \circ \nabla f_t$ | $A$     | $G$     | Total            |
|---------------|--------------------------|---------|---------|------------------|
| K-BFGS        | $O(d_i^2)$               | $O(d_o^2)$ | $O(d_i^2 + d_o^2 + d_i d_o)$ |
| K-BFGS(L)     | $O(d_i^2)$               | $O(pd_o)$ | $O(d_i^2 + d_i d_o + pd_o)$  |
| KFAC          | $O(d_i^2)$               | $O(d_o^2)$ | $O(d_i^2 + d_o^2 + d_i d_o)$  |
| Adam/RMSprop  | $O(d_i d_o)$             | $-$     | $O(d_i d_o)$                     |

### Table 2: Computation per iteration

| Algorithm     | Additional pass | Curvature | Step $\Delta W_t$          |
|---------------|-----------------|-----------|-----------------------------|
| K-BFGS        | $O(md_i d_o)$   | $O(md_i^2 + md_o + d_o^2)$ | $O(d_i^2 d_o + d_o^2 d_i)$ |
| K-BFGS(L)     | $O(md_i d_o)$   | $O(md_i^2 + md_o)$          | $O(d_i^2 d_o + pd_o d_i)$  |
| KFAC          | $O(md_i d_o)$   | $O(md_i^2 + md_o + \frac{1}{\tau}d_i^3 + \frac{1}{\tau}d_o^3)$ | $O(d_i^2 d_o + d_o^2 d_i)$ |
| Adam/RMSprop  | $-$             | $O(d_i d_o)$               | $O(d_i d_o)$                 |

**Experimental Results.** We tested K-BFGS and K-BFGS(L), as well as KFAC, Adam/RMSprop and SGD with momentum on three autoencoder problems, namely, MNIST [25], FACES, and CURVES, which are used in e.g. [22, 28, 29], except that we replaced the sigmoid activation with ReLU. See Section D in the appendix for a complete description on the autoencoder problems as well as the competing algorithms. As we are more interested in comparing different optimization methods, we focus on the training loss, rather than generalization performance.

Before we specify the hyper-parameters, since we can view Powell’s damping with $B = I$ as an LM damping, we choose $\mu_2 = \lambda_G$, where $\lambda_G$ denotes an LM damping for $G_t$. We then define $\lambda = \lambda_A \lambda_G$ as the overall damping term of our QN approximation. Instead of picking the values of $\lambda_A$, $\lambda_G$, we tune $\lambda$ while letting $\lambda_A = \lambda_G = \sqrt{\lambda}$. 

7
To obtain the results in Figure 1, we first did a grid-search on (learning rate, damping) pairs for all algorithms (except for SGD, whose grid-search was only on learning rate), where damping refers to $\lambda = \lambda_A \lambda_G$, $\epsilon$ for K-BFGS/K-BFGS(L)/KFAC, RMSprop/Adam, respectively. We then selected the best (learning rate, damping) pairs with the lowest training loss when terminated. The range for the grid-search and the best hyper-parameter values (as well as other fixed hyper-parameter values) are listed in Section D in the appendix. We then made 20 runs for the best hyper-parameters using different random seeds, and plotted the mean value of the 20 runs as the solid line and the standard deviation as the shaded area.\(^1\)

From Figure 1, our algorithms clearly outperformed the first-order methods, except for RMSprop/Adam on CURVES w.r.t CPU time. Our algorithms also performed better than KFAC in terms of CPU time.

To further demonstrate the robustness of our algorithms, we examined the loss under various hyper-parameters settings, which showed that they are stable under a fairly wide range of hyper-parameters. See Section D in the appendix for these and additional experimental results.

Figure 1: Comparison between algorithms on MNIST (left), FACES (middle), CURVES (right). The upper (lower) row depicts training progress versus CPU time (epoch), respectively. After each epoch, the loss from the whole training set is computed (the time for computing the loss is not included in the plots). For each problem, algorithms are terminated after the same amount of CPU time.

7 Conclusion

We proposed Kronecker-factored QN methods, namely, K-BFGS and K-BFGS(L), for training multi-layer feed-forward neural network models, that use layer-wise second-order information and require modest memory and computation resources. Experimental results indicate that our methods outperform or perform comparably to the state-of-the-art first-order and second-order methods. Our methods can also be extended to convolutional and recurrent NNs.

\(^1\) Results are obtained on a machine with 8 x Intel(R) Xeon(R) CPU @ 2.30GHz and 1 x NVIDIA Tesla P100.
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A Pseudocode for K-BFGS/K-BFGS(L)

Algorithm 4 gives pseudocode for K-BFGS/K-BFGS(L), which is implemented in the experiments. For details see Sections 3, 4, and Section C in the Appendix.

Algorithm 4 Pseudocode for K-BFGS / K-BFGS(L)

Require: Given initial weights \( \theta = \left[ \text{vec} (W_1)^\top, \ldots, \text{vec} (W_L)^\top \right]^\top \), batch size \( m \), learning rate \( \alpha \), damping value \( \lambda \), and for K-BFGS(L), the number of \((s, y)\) pairs \( p \) that are stored and used to compute \( H^l \) at each iteration
1: \( \mu_1 = 0.2, \beta = 0.9 \) \{set default hyper-parameter values\}
2: \( \lambda_A = \lambda_G = \sqrt{\lambda} \) \{split the damping into A and G\}
3: \( \nabla f_l = 0, A_l = E_t \left[ a_{l-1} (i) a_{l-1} (i)^\top \right] \) by forward pass, \( H^l_a = H^l_y = I \) \( (l = 1, \ldots, L) \) \{Initialization\}
4: for \( k = 1, 2, \ldots \) do
5: \( \) Sample mini-batch of size \( m \): \( M_k = \{ \xi_{k,i}, i = 1, \ldots, m \} \)
6: \( \) Perform a forward-backward pass over the current mini-batch \( M_k \) to compute \( \nabla f_l, a_l, h_l, \) and \( g_l \) \( (l = 1, \ldots, L) \) \{see Algorithm 1\}
7: for \( l = 1, \ldots, L \) do
8: \( \nabla f_l = \beta \nabla f_l + (1 - \beta) \nabla f_t \)
9: \( p_l = H^l_y \nabla f_l H^l_a \)
10: \{In K-BFGS(L), when computing \( H^l_g \left( \nabla f_l, H^l_a \right) \), LBFGS is initialized with an identity matrix\}
11: \( W_l = W_l - \alpha \cdot p_l \)
12: \( \) Perform another forward-backward pass over \( M_k \) to compute \( h^+_l, g^+_l \) \( (l = 1, \ldots, L) \)
13: for \( l = 1, \ldots, L \) do
14: \( \) \{Use damped BFGS or LBFGS to update \( H^l_g \) \{see Section 3\}\}
15: \( s^l_g = \beta \cdot s^l_g + (1 - \beta) \cdot \left( \hat{h}^l_a - h^l_a \right), y^l_g = \beta \cdot y^l_g + (1 - \beta) \cdot \left( g^l_f - g^l_f \right) \)
16: \( (\hat{s}^l_g, \hat{y}^l_g) = DD(s^l_g, y^l_g) \) with \( H = H^l_g, \mu_1 = \mu_1, \mu_2 = \lambda_G \) \{see Algorithm 3\}
17: \( \) Use BFGS or L-BFGS with \( (s^l_g, y^l_g) \) to update \( H^l_g \)
18: \{Use Hessian-action BFGS to update \( H^l_a \) \{see Section 4\}\}
19: \( A_l = \beta \cdot A_l + (1 - \beta) \cdot a_{l-1} a_{l-1}^\top \)
20: \( A^L_{LM} = A_l + \lambda_A I \)
21: \( s^l_a = H^l_a \cdot \bar{a}_{l-1}, y^l_a = A^L_{LM} \cdot s^l_a \)
22: \( \) Use BFGS with \( (s^l_a, y^l_a) \) to update \( H^l_a \)

B Convergence: Proofs of Lemmas 1-3 and Theorem 2

In this section, we prove the convergence of Algorithm 5, a variant of K-BFGS(L). Algorithm 5 is very similar to our actual implementation of K-BFGS(L) (i.e. Algorithm 4), except that

- we skip updating \( H^l_a \) if \( (\hat{s}^l_a)^\top \hat{y}^l_a < \mu_1 (\hat{y}^l_a)^\top H^l_a \hat{y}^l_a \) (see Line 16);
- we set \( H^l_a \) to the exact inverse of \( A^L_{LM} \) (see Line 21);
- we use decreasing step sizes \( \{\alpha_k\} \) as specified in Theorem 2;
- we use the mini-batch gradient instead of the momentum gradient (see Line 8).

To accomplish this, we prove Lemmas 1-3, which in addition to Assumptions AS.1-2, ensure that all of the assumptions in Theorem 2.8 in [39] are satisfied, and hence that the generic stochastic quasi-Newton (SQN) method, i.e. Algorithm 6, below converges. Specifically, Theorem 2.8 in [39] requires, in addition to Assumptions AS.1-2, the assumption

**AS. 4.** There exist two positive constants \( \kappa_1, \kappa \), such that \( \kappa^l \preceq H_k \preceq \kappa I, \forall k; \) for any \( k \geq 2 \), the random variable \( H_k \) depends only on \( \xi_{[k-1]} \).

In the following proofs, \( \| \cdot \| \) denotes the 2-norm for vectors, and the spectral norm for matrices.
Algorithm 5 K-BFGS(L) with DD-skip and exact inversion of $A^L_{TM}$

**Require:** Given initial weights $\theta = \left[ \text{vec}(W_1), \ldots, \text{vec}(W_L) \right]^T$, batch size $m$, learning rate $\alpha_k$, damping value $\lambda$, and the number of $(s, y)$ pairs $p$ that are stored and used to compute $H^l_g$ at each iteration.

1: $\mu_1 = 0.2, \beta = 0.9$ [set default hyper-parameter values]
2: $\lambda_A = \lambda_G = \sqrt{\lambda}$ [split the damping into $A$ and $G$]
3: $A_l(0) = E_{\xi} \left[ a_{l-1}(i)a_{l-1}(i)^T \right]$ by forward pass, $H^l_g(0) = H^l_g(0) = I (l = 1, \ldots, L)$ [Initialization]
4: for $k = 1, 2, \ldots$ do
5: Sample mini-batch of size $m$: $M_k = \{\xi_{k,i}, i = 1, \ldots, m\}$
6: Perform a forward-backward pass over the current mini-batch $M_k$ to compute $\nabla f_l$, $a_l$, $h_l$, and $g_l$ ($l = 1, \ldots, L$) (see Algorithm 1)
7: for $l = 1, \ldots, L$ do
8: $p_l = H^l_g(k - 1)\nabla f_l, H^l_g(k - 1)$, where $\nabla f_l = \nabla f_l$
9: {When computing $H^l_g(\nabla f_l H^l_g)$, LBFGS is initialized with an identity matrix}
10: $W_l = W_l - \alpha_k p_l$
11: Perform another forward-backward pass over $M_k$ to compute $h^+_l$, $g^+_l$ ($l = 1, \ldots, L$)
12: for $l = 1, \ldots, L$ do
13: {Use damped LBFGS with skip to update $H^l_g$ (see Section 3)}
14: $s^l_g = \beta \cdot s^l_g + (1 - \beta) \cdot (h^+_l - h_l), y^l_g = \beta \cdot y^l_g + (1 - \beta) \cdot (g^+_l - g_l)$
15: $(\tilde{s}^l_g, \tilde{y}^l_g) = \text{DD}(s^l_g, y^l_g)$ with $H = H^l_g(k - 1), \mu_1 = \mu_1, \mu_2 = \lambda_G$ [See Algorithm 3]
16: if $(\tilde{s}^l_g)^T \tilde{y}^l_g \geq \mu_1 (\tilde{y}^l_g)^T H^l_g \tilde{y}^l_g$ then
17: Use L-BFGS with $(\tilde{s}^l_g, \tilde{y}^l_g)$ to update $H^l_g(k)
18: {Use exact inversion to compute $H^l_g$}
19: $A_l(k) = \beta \cdot A_l(k - 1) + (1 - \beta) \cdot a_{l-1}a_{l-1}^T$
20: $A^L_{TM}(k) = A_l(k) + \lambda_A I_A$
21: $H^l_g(k) = \left(A^L_{TM}(k)\right)^{-1}$

Algorithm 6 SQN method for nonconvex stochastic optimization.

**Require:** Given $\theta_1 \in \mathbb{R}^n$, batch sizes $\{m_k\}_{k \geq 1}$, and step sizes $\{\alpha_k\}_{k \geq 1}$

1: for $k = 1, 2, \ldots$ do
2: Calculate $\nabla f_k = \frac{1}{m_k} \sum_{i=1}^{m_k} \nabla f(x_k, \xi_{k,i})$
3: Generate a positive definite Hessian inverse approximation $H_k$
4: Calculate $\theta_{k+1} = \theta_k - \alpha_k H_k \nabla f_k$

**Proof of Lemma 1:**

*Proof.* Because $A^L_{TM}(k) \succeq \lambda_A I_A$, we have that $H^l_u(k) \preceq \kappa_\lambda I_A$, where $\kappa_\lambda = \frac{1}{\lambda A}$.

On the other hand, for any $x \in \mathbb{R}^d$, by Cauchy-Schwarz, $\langle a_{l-1}(i), x \rangle^2 \leq \|x\|^2 \|a_{l-1}(i)\|^2 \leq \|x\|^2 (1 + \varphi^2 d_l)$.

Hence, $\|a_{l-1}a_{l-1}^T\| \leq 1 + \varphi^2 d_l$; similarly, $\|A_l(0)\| \leq 1 + \varphi^2 d_l$. Because $\|A_l(k)\| \leq \beta\|A_l(k - 1)\| + (1 - \beta)\|a_{l-1}a_{l-1}^T\|$, by induction, $\|A_l(k)\| \leq 1 + \varphi^2 d_l$ for any $k$ and $l$. Thus, $\|A^L_{TM}(k)\| \leq 1 + \varphi^2 d_l + \lambda_A$. Hence, $H^l_u(k) \succeq \kappa_\lambda I_A$, where $\kappa_\lambda = \frac{1}{1 + \varphi^2 d_l + \lambda_A}$.

**Proof of Lemma 2:**

*Proof.* To simplify notation, we omit the subscript $g$, superscript $l$ and the iteration index $k$ in the proof. Hence, our goal is to prove $\kappa \leq H = H^l_u(k) \succeq \kappa \lambda I$, for any $l$ and $k$. Let $(s_i, y_i) (i = 1, \ldots, p)$ denote the pairs
used in an LBFGS computation of \(H\). Since \((s_i, y_i)\) was not skipped, \(
abla_i^T H_i^{(i)} y_i \leq \frac{1}{\mu_i} \), where \(H_i^{(i)}\) denotes the matrix \(H_i\) used at the iteration in which \(s_i\) and \(y_i\) were computed. Note that this is not the matrix \(H_i\) used in the recursive computation of \(H\) at the current iterate \(\theta_k\).

Given an initial estimate \(H_0 = B_0^{-1} = I\) of \((G'_k(\theta_k))^{-1}\), the LBFGS method updates \(H_i\) recursively as

\[
H_i = \left( I - \rho_i s_i y_i^T \right) H_{i-1} \left( I - \rho_i y_i s_i^T \right) + \rho_i s_i s_i^T, \quad i = 1, \ldots, p, 
\]

(12)

where \(\rho_i = (y_i^T y_i)^{-1}\), and equivalently,

\[
B_i = B_{i-1} + \frac{y_i y_i^T}{s_i^T y_i} - \frac{B_{i-1} s_i y_i^T}{s_i^T B_{i-1} s_i}, \quad i = 1, \ldots, p, 
\]

where \(B_i = H_i^{-1}\). Since we use DD with skipping, we have that \(\frac{s_i^T s_i}{y_i^T y_i} \leq \frac{1}{\mu_i} \) and \(\frac{y_i^T H_i^{(i)} y_i}{s_i^T y_i} \leq \frac{1}{\mu_i} \). Note that we don’t have \(\frac{y_i^T H_i^{(i)} y_i}{s_i^T y_i} \leq \frac{1}{\mu_i} \), so we cannot directly apply (10). Hence, by (8), we have that \(|B_i| \leq |B_{i-1}| \left( 1 + \frac{1}{\mu_i} \right)\). Hence, \(|B| = |B_p| \leq |B_0| \left( 1 + \frac{1}{\mu_i} \right)^p = \left( 1 + \frac{1}{\mu_i} \right)^p. \) Thus, \(B \preceq \left( 1 + \frac{1}{\mu_i} \right)^p I, \)

\(H \succeq \left( 1 + \frac{1}{\mu_i} \right)^p I \equiv \bar{\kappa}_g I. \)

On the other hand, since \(\kappa_g\) is a uniform lower bound for \(H_i^{(i)}(k)\) for any \(k\) and \(l, \bar{\kappa}^{(i)} \geq \kappa_g I\). Thus,

\[
\frac{1}{\mu_i} \geq \frac{y_i^T H_i^{(i)} y_i}{s_i^T y_i} \geq \kappa_g \frac{y_i^T y_i}{s_i^T y_i} \Rightarrow \frac{y_i^T y_i}{s_i^T y_i} \leq \frac{1}{\mu_i \kappa_g}. 
\]

Hence, using the fact that \(|uv^T| = |u||v||v||\) for any vectors \(u, v, ||\rho_i s_i s_i^T|| = \rho_i ||s_i|| ||s_i|| = \frac{s_i^T s_i}{y_i^T y_i} \leq \frac{1}{\mu_i}, \)

\[
||H_i|| = || \left( I - \rho_i s_i y_i^T \right) H_{i-1} \left( I - \rho_i y_i s_i^T \right) + \rho_i s_i s_i^T || 
= ||H_{i-1} + \rho_i^2 (y_i^T H_{i-1} y_i) s_i s_i^T - \rho_i s_i y_i^T H_{i-1} - \rho_i H_{i-1} y_i s_i^T + \rho_i s_i s_i^T || 
\leq ||H_{i-1}|| + ||\rho_i^2 (y_i^T y_i) s_i s_i^T || + ||\rho_i s_i s_i^T || + ||\rho_i H_{i-1} y_i s_i^T || + ||\rho_i s_i s_i^T || 
\leq ||H_{i-1}|| + ||H_{i-1}|| \cdot ||\rho_i (y_i^T y_i) s_i s_i^T || + 2\rho_i ||s_i|| ||y_i^T H_{i-1}|| + \frac{1}{\mu_i} 
\leq ||H_{i-1}|| + ||H_{i-1}|| \cdot \frac{1}{\mu_i \kappa_g} \frac{1}{\mu_i} + 2\rho_i ||s_i|| ||y_i^T|| ||H_{i-1}|| + \frac{1}{\mu_i} 
\leq ||H_{i-1}|| \left( 1 + \frac{1}{\mu_i \kappa_g} \frac{1}{\mu_i} + \frac{2}{\sqrt{\mu_i \mu_i \kappa_g}} \right) + \frac{1}{\mu_i} 
= \mu ||H_{i-1}|| + \frac{1}{\mu_i}, \quad \text{where} \quad \mu = \left( 1 + \frac{1}{\sqrt{\mu_i \mu_i \kappa_g}} \right)^2 . 
\]

From the fact that \(H_0 = I, \) and induction, we have that \(||H|| \leq \bar{\mu}^p + \frac{\bar{\mu}^{p-1}}{\mu_i} \frac{1}{\mu_i} \equiv \bar{\kappa}_g. \)

\[\square\]

**Proof of Lemma 3:**

**Proof.** By Lemma 1, 2 and the fact that \(H_k = \text{diag}\{H_0^k(k-1) \otimes H_0^L(k-1), \ldots, H_0^L(k-1) \otimes H_0^L(k-1)\}. \)

**Proof of Theorem 2:**

**Proof.** To show that Algorithm 5 lies in the framework of Algorithm 6, it suffices to show that \(H_k\) generated by Algorithm 5 is positive definite, which is true since \(H_k = \text{diag}\{H_0^k(k-1) \otimes H_0^L(k-1), \ldots, H_0^L(k-1) \otimes H_0^L(k-1)\}\) and \(H_0^k(k-1)\) and \(H_0^L(k-1)\) are positive definite for all \(k\) and \(l\). Then by Lemma 3, and the fact that \(H_k\) depends on \(H_0^k(k-1)\) and \(H_0^L(k-1)\), and \(H_0^L(k-1)\) and \(H_0^L(k-1)\) do not depend on random samplings in the \(k\)th iteration, AS.4 holds. Hence, Theorem 2.8 of [39] applies to Algorithm 5, proving Theorem 2. \[\square\]
C  Powell’s Damped BFGS Updating

For BFGS and LBFGS, one needs $y^T s > 0$. However, when used to update $H^l_{y y}$, there is no guarantee that $(y^l_y)^T s^l_y > 0$ for any layer $l = 1, \ldots, L$. In deterministic optimization, positive definiteness of the QN Hessian approximation $B$ (or its inverse) is maintained by performing an inexact line search that ensures that $s^T y > 0$, which is always possible as long as the function being minimized is bounded below. However, this would be expensive to do for DNN. Thus, we propose the following heuristic based on Powell’s damped-BFGS approach [34].

**Powell’s Damping on $B$.** Powell’s damping on $B$, proposed in [34], replaces $y$ in the BFGS update, by $\tilde{y} = \theta y + (1 - \theta) Bs$, where

$$
\theta = \begin{cases} 
\frac{(1 - \mu)s^T B s}{s^T B s - \mu y^T s}, & \text{if } s^T y < \mu s^T B s, \\
1, & \text{otherwise}.
\end{cases}
$$

It is easy to verify that $s^T \tilde{y} \geq \mu y^T H y$.

**Powell’s Damping on $H$.** In Powell’s damping on $H$ (see e.g. [3]), $\tilde{s} = \theta s + (1 - \theta) H y$ replaces $s$, where

$$
\theta = \begin{cases} 
\frac{(1 - \mu)s^T H y}{y^T H y - \mu s^T H s}, & \text{if } s^T y < \mu y^T H y, \\
1, & \text{otherwise}.
\end{cases}
$$

This is used in lines 2 and 3 of the DD (Algorithm 3). It is also easy to verify that $s^T \tilde{y} \geq \mu y^T H y$.

**Powell’s Damping with $B = I$.** Powell’s damping on $B$ is not suitable for our algorithms because we do not keep track of $B$. Moreover, it does not provide a simple bound on $\frac{s^T \tilde{y}}{s^T y}$ that is independent of $|B|$. Therefore, we use Powell’s damping with $B = I$, in lines 4 and 5 of the DD (Algorithm 3). It is easy to verify that it ensures that $s^T \tilde{y} \geq \mu s^T y$.

Powell’s damping with $B = I$ can be interpreted as adding an Levenberg-Marquardt (LM) damping term to $B$. Note that an LM damping term $\mu$ would lead to $B \geq \mu I$. Then, the secant condition $\tilde{y}^T s = s^T B s \geq \mu s^T s$, which is the same inequality as we get using Powell’s damping with $B = I$.

C.1 Double Damping (DD)

Our double damping (Algorithm 3) is a two-step damping procedure, where the first step (i.e. Powell’s damping on $H$) can be viewed as an interpolation between the current curvature and the previous ones, and the second step (i.e. Powell’s damping with $B = I$) can be viewed as an LM damping.

Recall that there is no guarantee that $\frac{y^T H y}{s^T y} \leq \frac{2}{\mu}$ holds after DD. While we skip using pairs that do not satisfy this inequality, when updating $H^l_{y y}$ in proving the convergence of the K-BFGS(L) variant Algorithm 5, we use all $(s, y)$ pairs to update $H^l_{y y}$ in our implementations of both K-BFGS and K-BFGS(L). However, whether one skips or not makes only slight difference in the performance of these algorithms, because as our empirical testing has shown, at least 90% of the iterations satisfy $\frac{y^T H y}{s^T y} \leq \frac{2}{\mu}$, even if we don’t skip. See Figure 2 which reports results on this for K-BFGS(L) when tested on the MNIST, FACES and CURVES datasets, where hyper-parameters are the ones listed in Table 5.

D  Implementation Details and More Experiments

D.1 Description of Competing Algorithms

D.1.1 KFAC

We first describe KFAC in Algorithm 7. Note that $G_l$ in KFAC refers to the $G$ matrices in [29], which is different from the $G_l$ in K-BFGS.

D.1.2 Adam/RMSprop

We implement Adam and RMSprop exactly as in [24] and [21], respectively. Note that the only difference between them is that Adam does bias correction for the 1st and 2nd moments of gradient while RMSprop does not.
Figure 2: Fraction of the number of iterations in each epoch, in which the inequality $\frac{\gamma^T H_y s^T y}{n}$ holds (upper plots), and the average value of $\frac{\gamma^T H_y s^T y}{n}$ (lower plots) in each epoch. Legends in each plot assign different colors to represent each layer $l$.

**D.1.3 Initialization of Algorithms**

We describe how each algorithm is initialized in this part. For all algorithms, $\hat{\nabla} f$ is always initialized as zero. For second order information, we use a "warm start" for curvature when applicable, meaning that we will estimate curvature information before we start updating parameters. The information gathered is

- $A_l$ for K-BFGS and K-BFGS(L);  
- $A_l$ and $G_l$ for K-FAC;  
- $\nabla f \odot \nabla f$ for RMSprop;  
- Not applicable to Adam because of bias correction.

In other words, we will estimate the above quantities from the whole data set before we begin training. For simplicity, the time for "warm start" is not included in the plot.

Lastly, for K-BFGS and K-BFGS(L), $H_l^0$ is always initialized as identity matrix. $H_l^0$ is initialized as identity matrix in K-BFGS; for K-BFGS(L), when computing $H_l^0$ with LBFGS at every iteration, it is also initialized as identity matrix.
Algorithm 7 K-FAC

Require: Given $\theta_0$, batch size $m$, and learning rate $\alpha$, damping value $\lambda$, inversion frequency $T$

1: for $k = 1, 2, \ldots$ do
2: Sample mini-batch of size $m$: $M_k = \{\xi_{k,i}, i = 1, \ldots, m\}$
3: Perform a forward-backward pass over the current mini-batch $M_k$ (see Algorithm 1)
4: for $l = 1, 2, \ldots L$ do
5: $p_l = H_l^T \hat{\nabla} f_l H_l$
6: $W_l = W_l - \alpha \cdot p_l$
7: Perform another pass over $M_k$ with $y$ sampled from the predictive distribution
8: Update $A_l = \beta \cdot A_l + (1 - \beta) \cdot a_{l-1}^T a_{l-1}, G_l = \beta \cdot G_l + (1 - \beta) \cdot g_l g_l^T$
9: if $i \equiv 0 \pmod{T}$ then
10: Recompute $H_l^T = (A_l + \sqrt{\lambda} I)^{-1}, H_l^T = (G_l + \sqrt{\lambda} I)^{-1}$

D.2 Autoencoder Problems

Table 3 lists information about the three datasets, namely, MNIST, FACES, and CURVES. Even though we specify the training/testing splits, we focus on the training part in our experiments. Table 4 specifies the architecture of the 3 problems, where binary entropy $\mathcal{L}(a_{L, y}) = \sum_n [y_n \log a_{L,n} + (1 - y_n) \log(1 - a_{L,n})]$, MSE $\mathcal{L}(a_{L, y}) = \frac{1}{2} \sum_n (a_{L,n} - y_n)^2$. Besides the loss function in Table 4, we further add a regularization term $\frac{\eta}{2} ||\theta||^2$ to the loss function, where $\eta = 10^{-5}$.

| Dataset | # data points | # training examples | # testing examples |
|---------|--------------|---------------------|--------------------|
| MNIST   | 70,000       | 60,000              | 10,000             |
| FACES   | 165,600      | 103,500             | 62,100             |
| CURVES  | 30,000       | 20,000              | 10,000             |

| Dataset | Layer width & activation | Loss function |
|---------|--------------------------|---------------|
| MNIST   | [784, 1000, 500, 250, 30, 250, 500, 1000, 784] [ReLU, ReLU, ReLU, linear, ReLU, ReLU, ReLU, sigmoid] | binary entropy |
| FACES   | [625, 2000, 1000, 500, 30, 500, 1000, 2000, 625] [ReLU, ReLU, ReLU, linear, ReLU, ReLU, ReLU, linear] | MSE |
| CURVES  | [784, 400, 200, 100, 50, 25, 6, 25, 50, 100, 200, 400, 784] [ReLU, ReLU, ReLU, ReLU, ReLU, linear, ReLU, ReLU, ReLU, ReLU, ReLU, sigmoid] | binary entropy |

D.3 Specification of Hyper-parameters

In our experiments, we focus our tuning effort onto learning rate and damping. The range of the tuning values is listed below:

- learning rate $\alpha_k = \alpha \in \{1e-5, 3e-5, 1e-4, 3e-4, 1e-3, 3e-3, 1e-2, 3e-2, 1e-1, 3e-1, 1, 3, 10\}$.
- damping:
  - $\lambda$ for K-BFGS, K-BFGS(L) and K-FAC: $\lambda \in \{3e-3, 1e-2, 3e-2, 1e-1, 3e-1, 1, 3\}$.
  - $\epsilon$ for RMSprop and Adam: $\epsilon \in \{1e-10, 1e-8, 1e-6, 1e-4, 1e-3, 1e-2, 1e-1\}$.
  - Not applicable for SGD with momentum.

2 Downloadable at [http://yann.lecun.com/exdb/mnist/](http://yann.lecun.com/exdb/mnist/)
3 Downloadable at [www.cs.toronto.edu/~jmartens/newfaces_rot_single.mat](www.cs.toronto.edu/~jmartens/newfaces_rot_single.mat)
4 Downloadable at [www.cs.toronto.edu/~jmartens/digs3pts_1.mat](www.cs.toronto.edu/~jmartens/digs3pts_1.mat)
Based on the minimal loss value after termination, the value of best hyper-parameters used in Figure 1 are listed in Table 5. Besides the tuning hyper-parameters, we also list other fixed hyper-parameters with their values:

- Size of minibatch \( m = 1000 \), which is also suggested in [5].
- Decay parameter:
  - K-BFGS, K-BFGS(L): \( \beta = 0.9 \);
  - KFAC: \( \beta = 0.9 \);
  - RMSprop, Adam: Following the notation in [24], we use \( \beta_1 = \beta_2 = 0.9 \).
  - SGD with momentum: \( \beta = 0.9 \).
- Other:
  - \( \mu_1 = 0.2 \) in double damping (DD):
    We recommend to leave the value as default because \( \mu_1 \) represents the "ratio" between current and past, which is scaling invariant;
  - Number of \((s, y)\) pairs stored for K-BFGS(L) \( p = 100 \):
    It might be more efficient to use a smaller \( p \) for the narrow layers. We didn’t investigate this for simplicity and consistency;
  - Inverse frequency \( T = 20 \) in KFAC.

### D.4 Sensitivity to hyper-parameters

![Figure 3: Landscape of loss w.r.t hyper-parameters (i.e. learning rate and damping). The left, middle, right columns represent MNIST, FACES, CURVES, which are terminated after 500, 2000, 500 seconds (CPU time), respectively. The upper (lower) row is obtained with K-BFGS (K-BFGS(L)).](image)

\(^5\)The default value of \( \beta_2 \) recommended in [24] is 0.999. Hence, we also tested \( \beta_2 = 0.999 \), and obtained results that were similar to those presented in Figure 1 (i.e., with \( \beta_2 = 0.9 \)). For the sake of fair comparison, we chose to report the results with \( \beta_2 = 0.9 \).
Figure 3 shows the sensitivity of K-BFGS and K-BFGS(L) to hyper-parameter values (i.e. learning rate and damping). The $x$-axis corresponds to the learning rate $\alpha$, while the $y$-axis correspond to the damping value $\lambda$. Color corresponds to the loss after a certain amount of CPU time. We can see that both K-BFGS and K-BFGS(L) are robust within a fairly wide range of hyper-parameters.

To get the plot, we first obtain training loss with $\alpha \in \{1e-4, 3e-4, 1e-3, 3e-3, 1e-2, 3e-2, 1e-1, 3e-1, 1\}$ and $\lambda \in \{1e-2, 3e-2, 1e-1, 3e-1, 1\}$, and then draw contour lines of the loss within the above range.

D.5 Doubling the mini-batch for the gradient with almost no cost

Compared with other methods mentioned in this paper, our K-BFGS and K-BFGS(L) have an extra advantage of being able to double the size of minibatch for computing the stochastic gradient with almost no extra cost,
which might be of particular interest in a highly stochastic setting. To accomplish this, we can make use of the stochastic gradient computed at the second pass of the previous iteration, and average it with the stochastic gradient of the current iteration. In other words, say the size of minibatch is $m = 1000$, the above "double-grad" method enable us to have a stochastic gradient computed from 2000 data points at each iteration.

Some initial experiments are shown in Figure 4, where we compared our original K-BFGS ($m = 1000$) algorithm with its "double-grad" variants ($m = 500, 1000$, respectively). Even though "double-grad" does not help a lot in these experiments, our K-BFGS algorithm does perform stably across these different variants. These results indicate that there is a potential for further improvements; e.g., a finer grid search might identify hyper-parameter values that result in better performing algorithms.