Nonlinear Least Squares for Large-Scale Machine Learning using Stochastic Jacobian Estimates

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Abstract

For large nonlinear least squares loss functions in machine learning we exploit the property that the number of model parameters typically exceeds the data in one batch. This implies a low-rank structure in the Hessian of the loss, which enables effective means to compute search directions. Using this property, we develop two algorithms that estimate Jacobian matrices and perform well when compared to state-of-the-art methods.

1. Introduction

A major challenge in optimization of machine learning models is the large size of both; the large number of model parameters and the number of data points. Therefore, the use of higher derivative information whose complexity may scale quadratically with problem size typically has to be done in a careful manner (Bottou et al., 2018; Xu et al., 2020). Moreover, because very large data amounts may not be manageable all at once, even methods that use 1st order gradients only, usually randomly split the whole dataset into smaller blocks (minibatches). Once the data is appropriately prepared, the goal of an effective optimization algorithm is to fit the model accurately to the data by iteratively minimizing a loss objective function. A commonly used loss measure is the (mean) sum-of-squares (Higham & Higham, 2020). Since machine learning models are normally nonlinear, the resulting optimization problems are formulated as nonlinear least squares (NLLS) problems:

\[
\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{\gamma} \sum_{i=1}^{N} (m(\mathbf{w}; \mathbf{x}_i) - y_i)^2, \tag{1}
\]

where \( \gamma > 0 \) is a scaling value, \( m(\cdot; \mathbf{x}) \) is the machine learning model, \( (\mathbf{x}_i, y_i)_{i=1}^{N} \) are “(feature, label)” data pairs and \( \mathbf{w} \) are the optimization weights. Note that in (1) both \( n \) and \( N \) can be large. By splitting the data pairs into \( B \) minibatch blocks each containing \( L \) elements (i.e., \( N = BL \)) we define the indices \( i = bL + l \equiv i(b, l) \) for \( 1 \leq b \leq B \) and \( 1 \leq l \leq L \). Moreover, defining the residual at a data pair as \( r_i \equiv (m(\mathbf{w}; \mathbf{x}_i) - y_i) \) and the vector of residuals in a batch \( \mathbf{r}_b \equiv \left[ r_{i(1,b)}, r_{i(2,b)}, \ldots, r_{i(L,b)} \right]^\top \), the least squares objective is

\[
\sum_{i=1}^{N} (m(\mathbf{w}; \mathbf{x}_i) - y_i)^2 = \sum_{i=1}^{N} r_i^2 = L \sum_{b=1}^{B} \frac{1}{L} \mathbf{r}_b^\top \mathbf{r}_b. \tag{2}
\]

In the remainder we assume that for each batch the value of the objective \( \mathbf{r}_b^\top \mathbf{r}_b / L \) and its corresponding gradient \( \mathbf{g}_b \equiv \nabla_\mathbf{w} (\mathbf{r}_b^\top \mathbf{r}_b) / L \) are known.

2. Contribution

This work exploits the property that usually the number of data pairs \( L \) within a minibatch is smaller than the number of model parameters, i.e., \( L < n \). Combining this with the nonlinear least squares objective (2), we note that 2nd derivative matrices contain a low-rank structure that can be used for effective search direction computations. In particular, we describe two algorithms that approximate higher derivative information using a low memory footprint, and that have computational complexities, which are comparable to state-of-the-art first order methods. Other work on stochastic NLLS problems includes the computation of higher derivatives via a domain-decomposition process (Huang et al., 2021) or the analysis of noisy loss and residual values (Bergou et al., 2020). An initial backpropagation algorithm for the NLLS objective was developed in (Hagan & Menhaj, 1994). However, none of these works exploit the low rank structures in the loss objective.

3. Methods

Suppose that at a given batch \( 1 \leq b \leq B \) the loss \( \mathbf{r}_b^\top \mathbf{r}_b / L \) and its gradient \( \mathbf{g}_b \) are computed. We temporarily suppress the subscripts so that the residual vector and gradient are denoted \( \mathbf{r} \) and \( \mathbf{g} \), respectively. The 1st and 2nd derivatives of...
the loss are
\[
\nabla \left( \frac{r^\top r}{L} \right) = \frac{2}{L} \nabla r = g, \quad \text{and} \quad (3)
\]
\[
\nabla^2 \left( \frac{r^\top r}{L} \right) = \frac{2}{L} \nabla (\nabla r)^\top + \sum_{l=1}^{L} (\nabla^2 r_l)r_l. \quad (4)
\]
Throughout we will denote the Jacobian matrix by \( J \in \mathbb{R}^{n \times L} \) and the Hessian matrix as \( \nabla^2 (r^\top r/L) = H \). We define a new search direction at a current iteration \( k \) as the update to the weights: \( w^{(k+1)} = w^{(k)} + s \). Using Newton’s method the search direction is defined by the linear system
\[
H^{(k)} s_N = -g^{(k)}, \quad (5)
\]
where gradient, Jacobian and Hessian are evaluated at the current iteration, i.e., \( g^{(k)} = g(w^{(k)}) \), \( J^{(k)} = J(w^{(k)}) \), and \( H^{(k)} = H(w^{(k)}) \). For large \( n \) forming the Hessian matrix and solving with it is, however, not feasible. Thus we estimate the components in (4). First, note that the residuals near the solution are expected to be small and thus estimating the matrix \( \sum_{l=1}^{L} (\nabla^2 r_l)r_l \approx \frac{1}{\alpha} D \) with a diagonal \( D \) and scalar \( \alpha > 0 \) appears reasonable. For regular least squares problems setting \( D = 0 \) yields a Gauss-Newton method type, whereas \( D \neq 0 \) corresponds to a Levenberg-Marquardt type method (cf. (Nocedal & Wright, 2006)). In this work we develop methods that estimate the components of the Hessian, which are suited for large data in machine learning problems. In particular, we define search directions by the system
\[
\left( J^{(k)\top} J^{(k)} + \frac{1}{\alpha} D \right) s = -g^{(k)}, \quad (6)
\]
where the Jacobian \( J^{(k)} \) is approximated. Since \( L < n \) the matrix in parenthesis in (6) can be inverted using the Sherman-Morrison-Woodbury (SMW) inverse. Even so, computing the full Jacobian \( J^{(k)} \) is typically very expensive for large \( L \) and \( n \). Therefore, we describe two approaches for approximating \( J^{(k)} \) that enable effective computation of \( s \) in (6). Specifically, we derive representations of \( J^{(k)} \) based on the gradient/Jacobian relation in (3). In particular, the Jacobian matrices in this work approximate the relation \( \frac{2}{L} J^{(k)\top} r^{(k)} = g^{(k)} \).

\subsection*{3.1. Rank-1 Jacobian Estimate}

Let \( 1 \leq s \leq k \) denote an intermediate iteration. In our first approach we define the Jacobian estimate by a rank-1 matrix. More specifically, we represent an intermediate Jacobian in the form
\[
\hat{J}^{(s)}_1 = \frac{L}{2 \| r^{(s)} \|^2} g^{(s)} \cdot r^{(s)\top}, \quad (7)
\]
where the \( n + L + 1 \) coefficients \( \beta_i, \rho_i, \theta \) are to be determined. In order to satisfy the gradient/Jacobian relation \( \frac{2}{L} \hat{J}^{(s)}_1 r^{(s)} = g^{(s)} \) we deduce the form
\[
\hat{J}^{(s)}_1 = \begin{bmatrix} \beta_1 \rho_1 & \beta_2 \rho_2 & \cdots & \beta_L \rho_L \\ \beta_1 & \beta_2 & \cdots & \beta_L \\ \vdots & \vdots & \ddots & \vdots \\ \beta_1 \rho_L & \beta_2 \rho_L & \cdots & \beta_n \rho_L \end{bmatrix}, \quad (9)
\]
Note that in the rank-1 approximation of (8) the vectors of residuals \( r^{(1)} \cdots r^{(k)} \) need not be explicitly stacked, because the search direction in (6) uses the term \( \frac{L}{2} \hat{J}^{(s)}_1 J^{(k)\top} \), in which the residuals reduce to the inner product \( \sum_{s=1}^{k} r^{(s)\top} r^{(s)} = L f_k \).

\subsection*{3.2. Rank-L Jacobian Estimate}

For our second approach we use the rank-L representation
\[
\hat{J}^{(s)}_L = \text{diag}(g^{(s)}) P_1^\top P_2, \quad (9)
\]
where \( P_1 \) and \( P_2 \) are two random permutation matrices that rearrange the row and column ordering. In order to satisfy the relation \( \frac{L}{2} \hat{J}^{(s)}_L r^{(s)} = g^{(s)} \), the Jacobian estimate \( \hat{J}^{(s)}_L \) can be written as
\[
\hat{J}^{(s)}_L = \frac{L}{2} \text{diag}(g^{(s)}) P_1^\top R^{(s)} P_2, \quad (10)
\]
where $R^{(s)}$ is the rectangular matrix in (9) with elements

$$
\beta_i = \frac{1}{r_i}, \quad 1 \leq i < L \quad \text{and} \quad \beta_j = \frac{1}{r_L}, \quad L \leq j \leq n.
$$

We accumulate the intermediate estimates as to define the rank-L Jacobian as

$$
J_L^{(k)} = \sum_{s=1}^{k} \hat{J}_L^{(s)}. \quad (11)
$$

Finally, note that we do not form the Jacobians in (8) or (11) explicitly. Rather, we accumulate the information in $g^{(s)}, \|r^{(s)}\|^2$ and $\frac{g^{(s)}}{r_i}$. For instance, we represent $J_1^{(k)}$ by storing the vector $\sum_{s=1}^{k} g^{(s)}$ and the scalar $f^{(k)}$. For $J_L^{(k)}$ we store the non-zeros elements of (10) as a vector and subsequently accumulate these values in (11). Our methods are implemented in two algorithms for computing a new search direction.

4. Algorithms

This section describes algorithms for computing search directions based on our estimates of the Jacobian matrix. The model weights are updated according to $w^{(k+1)} = w^{(k)} + s^{(k)}$. Here the square of the diagonal matrix $d^{(k)} = \text{diag}(D^{(k)})$ is stored in a vector a squared accumulated gradients

$$
d^{(k)}^2 = \sum_{s=1}^{k} g^{(s)} \circ g^{(s)}, \quad (12)
$$

where $\circ$ represents element-wise multiplication. Similarly, $\div$ will stand for element-wise division and $\sqrt{}$ for the element-wise square root. Algorithm 1 implements the rank-1 estimate from Section 3.1.

Note that in Algorithm 1 part of the problem specifications, i.e. $B$ (number of batches) and $L$ (number of data pairs in a batch) determine the order of magnitude for the parameter $\delta$. Otherwise, we initialize $d^{(k)} = 1 \times 10^{-5} \text{ones}(n)$ and $\alpha = 5 \times 10^{-2}$. Moreover, if Jacobian accumulation were disabled, meaning that $J^{(k)} = 0$, then $s^{(k)} = 0$ and the search directions $s^{(k)}$ reduce to a basic version of the Adagrad algorithm (Duchi et al., 2011). The method of Section 3.2 can be implemented similarly in another algorithm. We will refer to the implementation of the rank-L Jacobian approximation as NLLSL.

Note that our algorithms can be implemented using element-wise multiplications, divisions, and square roots only, and are thus applicable to large problems.

5. Numerical Experiments

This section describes numerical experiments on three different optimization problems using the least squares loss. We compare our implementations of NLLS1 (Algorithm 1) and NLLSL with the widely used methods SGD, Adam (Kingma & Ba, 2015) and Adagrad (Duchi et al., 2011). The experiments are re-run 5 times for which the average loss evolution is plotted. On the x-axis are the number of epochs for a given experiment, which correspond to the number of data passes over the full dataset (each epoch the dataset is composed of $B$ batches with $L$ (feature, label) pairs). The algorithms are implemented in Python 3.7 with TensorFlow 2.4.0 (Developers, 2021) to compute the machine learning models and their derivatives. The experiments are carried out on a MacBook Pro @2.6 GHz Intel Core i7 with 32 GB of memory. The codes are freely available at

[https://github.com/johannesbrust/SNLLS](https://github.com/johannesbrust/SNLLS)

5.1. Experiment 1

This experiment compares 6 algorithms on a small classification problem using the Iris flower dataset. A fully connected network with three dense layers, softmax thresholding and relu activation is used. The dataset contains 3 different flower classes, which are characterized by 4 features. The number of optimization weights is $n = 193$, with data
sizes $L = 96$ and $B = 4$. Since the data is relatively small, we additionally include the “Full Jacobian” method, which explicitly computes the entire Jacobian in (3). Note however that unless $n$ and $L$ are small, computing full Jacobian matrices is not practical. Adam obtained good results using default TensorFlow parameters, while using a learning of 1.0 improved SGD. Adagrad used the same learning rate of 1.0 as SGD. The parameter in Algorithm 1 is $\delta = 0.8 \approx \frac{\sqrt{L/AB}}{3}$, and the outcomes are in Figure 1.

**Figure 1.** Comparison of 6 algorithms for the classification of 3 types of Iris plants (dataset: (Dua & Graff, 2017)). Observe that the “Full Jacobian” method reaches the lowest average loss as expected, since this method explicitly computes all Jacobian derivatives. However, the proposed rank-1 Jacobian approximation (NLLS1) achieves similar low losses, without explicitly computing the derivatives. The experiment outcomes are averaged over 5 runs.

### 5.2. Experiment 2

The movie recommendation dataset contains 100,000 (movie title, rating) pairs. A fully connected model with two dense layers and ReLU activation is used for rating predictions. Movie titles and ratings are embedded in two preprocessing layers of dimension 32. The total number of optimization weights is $n = 116,641$. The data sizes are $L = 8,192$ and $B = 13$. Since this problem is relatively large, computing full Jacobian matrices is not practical. Therefore the “Full Jacobian” method is not applicable in this experiment. However, all other algorithms are able to scale to the problem size. We use the default TensorFlow parameters for all algorithms, expect Adagrad which obtained better results with a learning rate of 0.1. We set the parameter $\delta = 20 \approx 2\sqrt{L/AB}$.

**Figure 2.** Comparison of 5 algorithms for training a movie recommender model on the MovieLens 100K dataset (Harper & Konstan, 2015). The proposed algorithm NLLS1 obtains the overall lowest losses. The outcomes are calculated as the average of 5 runs.

### 5.3. Experiment 3

In Experiment 3, the algorithms are applied to a large autoencoding model. The Fashion MNIST dataset of 60,000 $28 \times 28$ pixel images is used. The model consists of a dense layer with ReLU activation for the decoding (with embedding dimension 64) and dense layers with sigmoid activation for the decoding step. The total number of weights are $n = 101,200$ and the data consists of $L = 25,088$ and $B = 1,875$. We use the default TensorFlow parameters for Adam and set the learning rate to 50 for SGD and Adagrad. We set $\delta = 0.9 \approx 0.5\sqrt{L/AB}$.

**Figure 3.** Comparison of 5 algorithms for training an autoencoder on the Fashion MNIST dataset (Xiao et al., 2017). NLLS1 achieves the overall lowest loss values. The results are averaged over 5 runs.

### 6. Conclusions

This article develops algorithms that approximate Jacobian information in order to improve search directions in nonlinear least squares loss functions. By using the fact that the number of model parameters typically exceeds the number of data pairs in a batch of the dataset, we propose computationally effective methods for computing search directions. In numerical experiments, including large-scale applications, our proposed algorithms perform well when compared to the state-of-the-art such as Adam or Adagrad.
Stochastic NLLS

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