Large-Scale Classification using Multinomial Regression and ADMM

Samy Wu Fung∗† Sanna Tyrväinen†† Lars Ruthotto∗ Eldad Haber ††

Abstract

We present a novel method for learning the weights in multinomial logistic regression based on the alternating direction method of multipliers (ADMM). In each iteration, our algorithm decomposes the training into three steps; a linear least-squares problem for the weights, a global variable update involving a separable cross-entropy loss function, and a trivial dual variable update. The least-squares problem can be factorized in the off-line phase, and the separability in the global variable update allows for efficient parallelization, leading to faster convergence. We compare our method with stochastic gradient descent for linear classification as well as for transfer learning and show that the proposed ADMM-Softmax leads to improved generalization and convergence.

1 Introduction

Large-scale classification has a wide range of application areas such as data mining [20], neural signal processing [28], bioinformatics [56, 23] and text analysis [32]. Given a set of weights, the classification is commonly done using softmax regression (or multinomial logistic regression), where the data is separated in more than two mutually exclusive classes. The goal is to train a model efficiently leading to a satisfying success rate and good generalization, but large and complex datasets with many features make this computationally challenging.

In this paper, we propose an efficient learning algorithm for solving large-scale classification problems. We consider the softmax classifier and train it by solving an unconstrained optimization problem with cross-entropy as the loss function and an $\ell_2$-regularization for the weights to avoid over-fitting the data. In this case, there are a variety of algorithms that can be used to train the classifiers, e.g., steepest descent [24], and perhaps more common in cases with many examples, stochastic gradient descent (SGD) [42, 19]. However, parallelization of these methods is not trivial as methods like SGD are sequential; this can result in very slow convergence when large amounts of data are available.

To facilitate parallelization, we reformulate the unconstrained optimization problem into a constrained one whose objective function is separable along the examples and whose coupling is enforced by the constraints. We consider the alternating direction method of multipliers (ADMM) to decompose the constrained optimization problems into three subproblems that can be solved efficiently. Each iteration of our scheme consists of a weight-update that involves solving a least-squares (LS) problem, a global variable update that involves a cross-entropy problem that is separable along the examples, and a trivial dual update variable. The LS problem arising from the weights can be efficiently solved using direct or iterative solvers [10, 30]. The convex and smooth softmax problem arising from the global variable update can also be solved efficiently since the separability along examples renders it highly parallelizable. Finally, the dual variable update is a trivial step requiring only a matrix-vector product. More details can be found in Section 5.

The inspiration for our classifier comes from the application of ADMM to $\ell_1$-regularized linear inverse problems, also known as lasso [54, 31] and basis pursuit [4]. Here, ADMM breaks the lasso problem into two subproblems: one containing a smooth least squares problem, and the other containing a decoupled non-linear, non-smooth term which allows for efficient use of soft thresholding [7]. Our problem can be similarly divided into a least squares problem and many decoupled smaller problems for the nonlinear cross-entropy loss minimization.

We test our method on the MNIST [21, 22] and CIFAR-10 [17] datasets, which are not linearly separable. To improve accuracy and generalization, we adjust the inputs for the MNIST dataset by seeking a hyperplane in an enlarged data space by propagating our input data through a fixed random layer. We also use transfer learning [27], where we propagate our data through a network that has been pre-trained on a similar data set. In particular, we use feature
2 Multinomial Logistic Regression

In this section, we briefly review the mathematical formulation for multinomial logistic regression. Let \( \mathbf{Y} = [\mathbf{y}_1 \mathbf{y}_2 \cdots \mathbf{y}_{n_c}] \in \mathbb{R}^{n_x \times n_f} \) be the feature matrix, and \( \mathbf{C} = [\mathbf{c}_1 \mathbf{c}_2 \cdots \mathbf{c}_{n_c}] \in \mathbb{R}^{n_x \times n_c} \) the label matrix, where \( n_x, n_f, \) and \( n_c \) are the number of examples, features, and class labels, respectively. Each row \( \mathbf{c}_k \) denotes the probability of labels for its corresponding sample \( \mathbf{y}_k \).

Given data \( \mathbf{Y} \), we can predict the class labels of the data using the softmax classifier function

\[
\mathbf{C}_{\text{pred}} = h_{\mathbf{W}}(\mathbf{Y}) = \text{diag} \left( \frac{1}{\exp(\mathbf{Y} \mathbf{W}) \mathbf{e}_{n_c}} \right) \exp(\mathbf{Y} \mathbf{W}),
\]

where \( \mathbf{e}_{n_c} \in \mathbb{R}^{n_c} \) is the vector of all ones. The cross-entropy loss function quantifies the between the true probabilities \( \mathbf{C} \) and the predicted probabilities \( h_{\mathbf{W}}(\mathbf{Y}) \). Here \( \odot \) denotes the Hadamard product, i.e., element-wise product. From the inner sum of the second term in (2), we can see that the weights are coupled for each example. This lack of separability leads to difficulties in the parallelization of classical optimization algorithms used to minimize the entropy loss function. The problem can thus be very challenging computationally for large amounts of high-dimensional data.

In addition to solving the optimization efficiently, we also wish to learn a model that generalizes well on unseen data. We do this by adding regularization in order to avoid overfitting. In particular, we solve the multinomial logistic regression model

\[
\min_{\mathbf{W}} \mathcal{F}(\mathbf{W}) = \Phi(\mathbf{C}, \mathbf{Y} \mathbf{W}) + \alpha \mathbf{R}(\mathbf{W}),
\]

where \( \alpha > 0 \) is a regularization parameter that balances the minimization of the loss and the regularity of the solution. We assume \( \alpha \) is chosen by the user.

In general, there is no closed-form solution to (3), however, the objective function is convex and differentiable so that gradient-based iterative optimization algorithms including SGD \( [42] \) can be used to solve it.

2.1 Related Work

Multinomial regression is a central problem in many task, which has led to many numerical methods tailored to specific data structures. A common thread are the efforts to parallelize the solution of (5) over the examples, or classes. Note that the problem is not trivially parallelizable since, as previously mentioned, the log-sum-exp term in (2) couples the weights through all the examples.

One class of methods is based on deriving separable upper bounds on the objective function. For example, \( [11] [14] \), use an upper bound based on the first-order concavity property of the log-function. This approach gives a new optimization problem that is not convex, but where the objective is separable across the weights associated with the different classes. There are other possible upper-bounds for a softmax function, such as a quadratic upper bound and a product of sigmoids. Detailed comparison of these and analytical solutions in a Bayesian setting can be found in \( [11] \). Gopal and Yang \( [11] \) use the concavity bound to solve multinomial logistic regression in parallel, and prove that their iterative optimization of the bounded objective converges to the same optimal solution as the unbounded original model. Related to the concavity bound, Fagan & Iyengar \( [9] \) and Raman et al. \( [29] \) use convex conjugate of negative log to reformulate the problem as a double-sum that can be solved iteratively with SGD.
method presented in their paper. The approach is inspired does not compare in computation efficiency to the principal be solved in parallel, but the authors state that this approach challenging log-sum term. The new optimization problem can be solved separately. That is, the new global auxiliary parameter of ADMM is implanted only on the challenging log-sum term. The new optimization problem can be solved in parallel, but the authors state that this approach does not compare in computation efficiency to the principal method presented in their paper. The approach is inspired by the work of Boyd et al. [2] who solve sparse logistic regression problem parallel by splitting it across features with ADMM.

Taylor et al. [33] introduced an approach for solving the non-convex problem of training neural networks using ADMM and Bregman iteration. Their examples concentrate on binomial regression which allows them to use quadratic loss function and closed form solutions for each iteration step. Another related approach is the method of auxiliary coordinates (MAC) [3]. In MAC new variables are introduced to decouple the problem. Unlike ADMM, however, MAC breaks the deep nesting, i.e. function compositions, in the objective function with the new parameters.

Sparse logistic regression has been proposed as a method for feature selection in large-scale classification problems as sparsity can help identify the most important features, which avoids over-fitting and can reduce the computing time. The sparsity is generally forced with $\ell_1$-regularization, but $\ell_1$ is non-differentiable, leading to difficulties in training. There are different approaches to solve this, like interior point-method [15], iterative shrinkage method [12] and hybrid algorithm [31]. See, for example, Krishnapuram et al. [16] or the survey by Yuan et al. [40].

3 ADMM-Softmax

Motivated by the discussions in the previous section, we derive a novel ADMM algorithm to solve (3); see [2] for an excellent introduction. Our main idea, is to split the multinomial regression problem into a regularized least squares problem and a separable smooth convex optimization problem, noting that efficient solvers exist for both subproblems. For ease of presentation, we use $\ell_2$-regularization since it allows us to have a closed-form least-squares solution when updating the weights, however, our method can easily be extended to other regularizers. In particular, we relax (3) by introducing a global auxiliary variable $Z \in \mathbb{R}^{n_e \times n_c}$ and reformulate it as

$$\arg \min_{W,Z} \Phi (C, Z) + \frac{\alpha}{2} \|L (W - W_{\text{ref}})\|^2_F$$

s.t. $Z - YW = 0.$

The second term is a Tikhonov regularizer [26, 25, 35] where $L$ is the regularization operator.

To solve (4) using the ADMM algorithm we first consider the Lagrangian

$$\mathcal{L}_\rho (W, Z, X) = \Phi (C, Z) + e_n^T (X \odot (Z - YW)) e_n + \frac{\rho}{2} \|Z - YW\|^2_F + \frac{\alpha}{2} \|L (W - W_{\text{ref}})\|^2_F,$$

where $X \in \mathbb{R}^{n_e \times n_c}$ is the estimate of the Lagrange multiplier, $\rho \geq 0$ is the penalty parameter, and $e_n, e_{n_c} \in \mathbb{R}^{n_e}$ are vectors of all ones. The ADMM algorithm aims to finding the saddle point of the Lagrangian via the following iterations:

$$W^{(k+1)} = \arg \min_W \mathcal{L}_\rho (W, Z^{(k)})$$

$$Z^{(k+1)} = \arg \min_Z \mathcal{L}_\rho (W^{(k+1)}, Z)$$

$$X^{(k+1)} = X^{(k)} + \rho (Z^{(k+1)} - YW^{(k+1)}).$$

These iterations can be written more explicitly using the scaled ADMM algorithm (see [2]) as

$$W^{(k+1)} = \arg \min_W \frac{\rho}{2} \|Z^{(k)} - YW + U^{(k)}\|^2_F + \frac{\alpha}{2} \|L (W - W_{\text{ref}})\|^2_F$$

$$Z^{(k+1)} = \arg \min_Z \Phi (C, Z) + \frac{\rho}{2} \|Z - YW^{(k+1)} + U^{(k)}\|^2_F$$

$$U^{(k+1)} = U^{(k)} + \left(Z^{(k+1)} - YW^{(k+1)}\right),$$

where $U = (1/\rho)X$ is the scaled Lagrange multiplier. The subproblem (7) involves a regularized least-squares, and a global variable step (8), which is convex and separable along the examples, leading to trivial parallelization (see Sec. 3.2).

We note that using a different regularization in the original optimization problem (3) would only impact the least-squares subproblem (7) and the global variable minimization step (8) would stay the same. There are many efficient ways to solve least-square problem with different types regularizations terms. A good example would be using $\ell_1$-regularization, which renders (7) a lasso problem. In this case, there are many established solvers that efficiently solve the lasso problem (see Sec. 2.1) that can be used in our framework.

As for the stopping criteria, we follow [2] and define the
squared norms of the primal and dual residuals to be
\[ \|r^{(k+1)}\|_2^2 = \|Z^{(k+1)} - YW^{(k+1)}\|_F^2 \quad \text{and} \quad \|s^{(k+1)}\|_2^2 = \|\rho Y^T(Z^{(k+1)} - Z^{(k)})\|_F^2, \]
respectively. The termination criterion is satisfied whenever
\[ \epsilon_{pri}^{(k)} = \sqrt{n_e n_c} \epsilon_{abs} + \epsilon_{ref} \max \left\{ \|Z^{(k)}\|_2, \|YW^{(k)}\|_F \right\}, \]
\[ \epsilon_{dual}^{(k)} = \sqrt{n_e n_c} \epsilon_{abs} + \epsilon_{ref} \|U^{(k)}\|_F, \]
where \( \epsilon_{ref} > 0 \) and \( \epsilon_{abs} > 0 \) are the relative and absolute tolerances chosen by the user.

### 3.1 Solving the LS problem

Updating the weight matrix \( W \) requires solving (7). This is equivalent to solving normal equations
\[ (\rho Y^T Y + \alpha L^T L) W = \rho Y^T Z + U + \alpha L^T L W_{ref}. \]
Note that the coefficient matrix is not iteration-dependent. Thus, depending on the number of features, the matrix can be factorized once and quickly applied.

In the case that coefficient matrix cannot be explicitly constructed, we can use iterative methods, e.g., CGLS [10] with, e.g., the incomplete Cholesky factorization [10] as a preconditioner. Another option is to use sample average approximation [14] to reduce the dimension of the problem and pre-compute a factorization in the offline phase, e.g., thin QR or Cholesky [10], leading to trivial solves throughout the optimization scheme. We note that these are only some approaches for solving (12), and that a myriad of additional options exist [10, 30].

### 3.2 Global Variable Update

The global variable minimization step [8] can be written as
\[ \Psi(Z) = -e_{n_e}^T (C \odot Z) e_{n_e} \]
\[ + \sum_{i=1}^{n_e} \left( -c_i^T Z_i + \log(\exp(Z_i)) e_{n_e} \right) + \frac{\rho}{2} \|Z - Z_{ref}\|_F^2, \]
\[ = \sum_{i=1}^{n_e} \left( -c_i^T Z_i + \log(\exp(Z_i)) e_{n_e} \right) + \frac{\rho}{2} \|Z_i - Z_{ref,i}\|_2^2, \]
where \( Z_{ref} = YW - U \), and the vectors \( \{Z_1, Z_2, \ldots, Z_{n_e}\} \) correspond to the rows of the matrix \( Z \). For brevity, we maintain the matrix notation.

We can then write the gradient as
\[ \nabla Z \Psi (Z) = -C + \exp(Z) \odot \left( \frac{1}{\exp(Z) e_{n_e}} e_{n_e}^T \right) \]
\[ + \rho (Z - Z_{ref}), \]
and the product of the Hessian times a matrix \( S \in \mathbb{R}^{n_e \times n_e} \) as
\[ \nabla^2 Z \Psi (Z) S = \left( \frac{\exp(Z)}{\exp(Z) e_{n_e} e_{n_e}^T} \right) \odot S \]
\[ - \left( \frac{\exp(Z)}{(\exp(Z) e_{n_e})^2} e_{n_e}^T \right) \odot \left( (\exp(Z) \odot S) e_{n_e} e_{n_e}^T \right), \]
where the squaring in the denominator of the second term is applied component-wise. Unlike in (2), the objective function in (13) is separable along the examples, allowing for easy parallelization. In particular, the gradients and Hessians can be computed locally and independently for different examples, leading to reduced runtimes. Finally, ADMM-Softmax provides us with additional flexibility since we can solve [8] using any classical gradient-based optimization algorithm.

### 3.3 Computational Costs and Convergence

For the ADMM-Softmax formulation, the global variable update [8] can be solved using the Newton-PCG method [17] (as we do in our experiments), and the Hessian matrix-matrix product used in (15) only requires performing a Hadamard product with \( \exp(Z) \), which is in the order of \( O(n_e n_c) \). Assuming \( n_w \) workers are available, the cost for each Hessian matrix-matrix product seen in (15) is in the order of about \( O \left( \frac{n_e n_c}{n_w} \right) \) per worker, leading to very fast computations of the global variable update. The main computational bottleneck in ADMM-Softmax thus lies in solving the LS problem (7), for which there are ample options for solving efficiently [10]. When a factorization of the coefficient matrix can be performed in the off-line phase, e.g., Cholesky or thin QR, we can trivially solve LS throughout the optimization.

Finally, it has been shown that the ADMM algorithm converges linearly for convex problems with existing solutions regardless of the initial choice \( \rho^{(0)} \) [8]. If (7) is solved inexactly, ADMM still converges under additional assumptions [13]. In our case, the cross-entropy loss function with the softmax classifier is convex, and thus we are guaranteed convergence with ADMM-Softmax.
4 Numerical Experiments

In this section, we demonstrate the potential of our proposed ADMM-Softmax on the MNIST and CIFAR-10 datasets. For both datasets, we compare the performance of the proposed ADMM-Softmax and SGD. Our experiments are coded in MATLAB using the Meganet deep learning package [38]. Moreover, our ADMM-Softmax framework is coded as an extension of the package. We perform all of our experiments on a shared memory computer operating Ubuntu 14.04 with 2 Intel Xeon E5-2670 v3 2.3 GHz CPUs using 12 cores each, and a total of 128 GB of RAM.

4.1 Setup

4.1.1 MNIST

The MNIST database consists of 60,000 grey-scale handwritten images of digits ranging from 0 to 9. [21, 22] Here, we set 50,000 examples for training our digit-recognition system and the remaining 10,000 as validation data. Each digit is normalized with size $28 \times 28$, or with 784 pixel in total as the features. Some examples are shown in Fig. 1.

Since the data is not linearly separable, we seek a hyperplane in an enlarged subspace obtained by a non-linear transformation to the original variables. Specifically, we propagate the data through a single fixed hidden layer where we apply a $3 \times 3$ random convolution filter with 9 channels:

$$Y_{\text{prop}} = \tanh(YK),$$

where $K \in \mathbb{R}^{n_f \times m}$ is a block-circulant matrix with circulant block (BCCB) convolution matrix [?] and $m$ denotes the size of the new feature space. The transformed feature matrix has dimensions $50,000 \times 7057$, where each row now consists of 9 images. An illustration of the feature transformation is shown in Figure 2.

We compare two algorithms, our proposed ADMM-Softmax and SGD. In SGD, we use Nesterov momentum with minibatch size 30, and learning rate $l_r = l_{r_0}/\sqrt{c_e}$, where $c_e$ is the current epoch, $l_{r_0} = 10^{-2}$ is the initial learning rate. Here, we choose the initial learning rate and minibatch sizes by performing a grid-search on $[10^{-8}, 10^3]$ and $[1, 100]$, respectively. The initial learning rate grid-search is done logarithmically whereas the minibatch size grid-search is performed uniformly. In the ADMM-Softmax, we use initial $\rho = 10^{-2}$, with absolute and relative tolerance described in (10) to be $10^{-3}$. To solve the LS system, we compute a Cholesky factorization in the off-line phase, which for this experiment took about 0.3 seconds. To solve (8), we use the Newton-PCG method from the Meganet package using a maximum 30 iterations and a gradient norm stopping tolerance of $10^{-1}$. The inner Newton system is solved using the preconditioned conjugate gradients (PCG) with a maximum of 10 inner iterations and stopping tolerance of $10^{-1}$.

For both methods, we use the Laplace operator as the regularization operator $L$ to enforce smoothness of the images, and set reference weights to $W_{\text{ref}} = 0$. We set regularization parameter to $\alpha = 10^{-1}$ for SGD and $\alpha = 1$ for ADMM-Softmax, which were chosen based on the best results from performing a logarithmic grid-search on $[10^{-8}, 10^3]$.

4.1.2 CIFAR-10

The CIFAR-10 dataset [17] consists of 60,000 $32 \times 32$ RGB-valued images in 10 classes. Here, we have 50,000 examples of data for training and 10,000 for validation. The images belong to one of the following 10 classes: airplane, automobile, bird, cat, deer, dog, frog, horse, ship, and truck.

For this dataset, we increase the feature space by propagating our feature matrix through a pre-trained AlexNet [18] on the ImageNet dataset [5] from MATLAB’s deep neural networks toolbox. In particular, we remove the last fully-connected layer and treat the rest AlexNet as a fixed feature extractor for the new dataset. In this case, the propagated feature matrix has dimensions $50,000 \times 4096$.

As for the optimization, we maintain the same setup as the MNIST data set. We perform the same grid-search on the learning rate and minibatch sizes as in MNIST and report the parameters that led to the best results. In SGD, we obtain the best results with learning rate as $l_{r_0} = 10$ and minibatch size 40. In ADMM-Softmax, we choose the

![Figure 1. Example of 30 hand-written images obtained from the MNIST data set](image1)

![Figure 2. Feature transformation of a single image in the original feature matrix.](image2)
penalty parameter as $\rho = 10^{-1}$. Since the propagated features no longer correspond to images in this case, we use the identity as the regularization operator with $\alpha = 10^{-1}$ for SGD and $\alpha = 1$. As before, we chose the $\alpha$ and $\rho$ that led to the best results for each algorithm after performing a grid-search on $[10^{-8}, 10^3]$ for each algorithm, respectively.

4.2 Results

In Fig. 4 we show the performance of both algorithms applied to MNIST and CIFAR-10. To make a fair comparison between both algorithms, we compare the performance based on the runtime of each algorithm - this is because an iteration of ADMM-Softmax requires more computational work than an iteration of SGD. We let both algorithms run for a maximum of 500 seconds, and as can be seen, we obtain faster convergence with ADMM-Softmax. We note that we did not use any parallelization in any of these experiments, however, further speed ups are to be expected when the global variable step is performed in parallel.

5 Conclusion

We propose a simple and efficient algorithm for solving large-scale classification problems. To this end, we reformulate the traditional softmax regression problem consisting of an unconstrained coupled optimization into a constrained one where the objective function is decoupled and the coupling is enforced by the constraints. The new formulation is solved by the alternating direction method of multipliers (ADMM) which breaks down the problem into three simpler steps consisting of a least-squares (LS), a separable softmax problem, and a trivial dual variable update per outer iteration. ADMM-Softmax allows for plenty of flexibility since the resulting separable softmax problem can be solved using any classical optimization algorithm efficiently and in parallel (see Sec. 3).

Our numerical results show improved convergence when compared to SGD for the MNIST and CIFAR-10 datasets. We refrain from solving these problems in parallel since the datasets were relatively small; however, since our proposed ADMM-Softmax contains a highly parallelizable step, further benefits are to be expected for large datasets where parallelization is necessary.

We note that better accuracies, especially for the CIFAR-10 dataset, could be achieved if we fine-tune the parameters of pre-trained AlexNet [39]. To this end, our method can accelerate block-coordinate algorithms that alternate between updating the network weights and the classifier. This is a direction of our future work.

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