Abstract

Multinomial logistic regression, also known by other names such as multiclass logistic regression and softmax regression, is a fundamental classification method that generalizes binary logistic regression to multiclass problems. A recently work [5] proposed a faster gradient called quadratic gradient that can accelerate the binary logistic regression training, and presented an enhanced Nesterov’s accelerated gradient (NAG) method for binary logistic regression. In this paper, we extend this work to multiclass logistic regression and propose an enhanced Adaptive Gradient Algorithm (Adagrad) that can accelerate the original Adagrad method. We test the enhanced NAG method and the enhanced Adagrad method on some multiclass-problem datasets. Experimental results show that both enhanced methods converge faster than their original ones respectively.

1 Introduction

Logistic regression (LR) is a classical model in machine learning applied for estimating conditional probabilities. This model has been widely used in a variety of specific domains such as health and finance, both for binary classification and multi-class problems. Although the theory for binary logistic regression is well developed [6], its multiclass extension is much less studied.

Multinomial logistic regression is a decision-making task where examples consist of a feature vector and a categorical class label with more than two choices. For each input of a feature vector representing the example to be classified, the multinomial logistic regression model is expected to output a prediction of probabilities of the label of the example. The model performance can be measured by their log-loss and accuracy.

Motivated by its widely used in real-world applications, effects have been made to find efficient methods for multiclass LR. Böhning [2] proposed a fixed good lower bound for multiclass LR. Our work is most related to Chiang [5] and can be seen as the following work to [5]. Chiang [5] proposed a faster gradient variant named quadratic gradient and presented an enhanced NAG method for binary LR with the help of quadratic gradient. This work extends binary LR to multiclass LR problems and presents the enhanced Adagrad method for the multiclass LR.

2 Preliminaries

Chiang [5] proposed a faster gradient variant named quadratic gradient and claimed that quadratic gradient can unite the first-order gradient method and the second-order Newton’s method. This faster gradient variant can be seen as an extension of the simplified fixed Hessian [4] and be built by constructing a diagonal substituted matrix that suffices the convergence condition of the fixed Hessian method [3].
Chiang’s Quadratic Gradient  

Supposing that a differentiable scalar-valued function \( F(x) \) has its gradient \( g \) and Hessian matrix \( H \). To maximize the function \( F(x) \), we try to find a good lower bound matrix \( \tilde{H} \leq H \); To minimize the function \( F(x) \), we need to find a good upper bound \( \bar{H} \) such that \( H \leq \bar{H} \). Here “\( \leq \)” is in the Loewner order and \( A \preceq B \) means that \( A - B \) is non-negative. We first build a diagonal matrix \( \tilde{B} \) from the good bound matrix \( \bar{H} \) as follows:

\[
\tilde{B} = \begin{bmatrix}
\frac{1}{\varepsilon + \sum_{i=0}^{n} |h_{0i}|} & 0 & \cdots & 0 \\
0 & \frac{1}{\varepsilon + \sum_{i=0}^{n} |h_{1i}|} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \frac{1}{\varepsilon + \sum_{i=0}^{n} |h_{ni}|}
\end{bmatrix},
\]

where \( h_{ji} \) is the elements of the matrix \( \bar{H} \) and \( \varepsilon \) an arbitrarily small positive number.

The quadratic gradient \( G \) for function \( F(x) \) is defined as \( G = \tilde{B} \cdot g \) and have the same dimension as the naive gradient \( g \). The way to use it is much the same as the first-order gradient method, except that we need to replace the naive gradient with the quadratic gradient and increase the learning rate by 1. For example, \( x = x + \eta G \) and \( x = x - \eta G \) to maximise the function \( F(x) \) and minimise the function \( F(x) \) respectively. Note that the new learning rate \( \eta \) should be no less than 1 for efficiency and convergence speed. Moreover, sophisticated gradient (descent) methods such as NAG and Adagrad can be applied in practice to improve the performance further.

Bonte and Vercauteren [4] presented the Simplified Fixed Hessian (SFH) method for binary LR by constructing a simplified diagonal fixed Hessian from the good lower bound matrix proposed by Böhrnig and Lindsay [3]. In real-world applications, it is not easy to find the fixed Hessian matrix, and sometimes it even does not exist or is not a good lower bound of the Hessian matrix. In these cases, we can build the quadratic gradient directly from the Hessian matrix itself, rather than struggling to find a fixed Hessian substitute. The quadratic gradient doesn’t stick to a “fixed” replaced matrix but only adheres to a good bound matrix. Letting the Hessian matrix \( \bar{H} \) itself be the good bound \( \bar{H} \), we can see that the diagonal matrix \( \tilde{B} \) built directly from \( \bar{H} \) suffices the theory of the fixed Hessian method.

For maximising \( F(x) \), we need to find a matrix \( \bar{H} \) such that \( \bar{H} \leq H \) to follow the (simplified) fixed Hessian method. Chiang [5] has already proved that the above given \( \tilde{B} \) is a lower bound to \( \bar{H} \): \( \tilde{B} \leq \bar{H} \leq H \).

The problem of minimising \( F(x) \), however, can be seen as to maximize the function \( G(x) = -F(x) \). Function \( G(x) \) has its gradient \(-g\) and Hessian matrix \(-H\). To maximize \( G(x) \), we need to find a matrix \( \bar{H} \) such that \( \bar{H} \preceq -H \) and get the iteration: \( x = x + (\bar{H})^{-1}(-g) \) or \( x = x - (\bar{H})^{-1}g \). Namely, we need to find the lower bound \( \bar{H} \) of \(-H\) or the upper bound \(-H\) of \( H \) such that \( -\bar{H} \geq H \) and then build the quadratic gradient from \( \bar{H} \) or \(-\bar{H} \). The constructions of quadratic gradient for \( H \) and \(-\bar{H} \) result in the same quadratic gradient.

In conclusion, to calculate the quadratic gradient, we can find a matrix \( \bar{H} \leq H \) for the maximization problem or a matrix \( \bar{H} \geq H \) for the minimization problem. A better way is to construct the \( \tilde{B} \) from the Hessian matrix \( H \) directly and then try to find a good upper bound for each diagonal element of \( \tilde{B} \) if there exists one.

3 Technical details

Given an dataset matrix \( X \in \mathbb{R}^{n \times (1+d)} \), each row of which represents a record with \( d \) features plus the first element 1. The outcome \( Y \in \mathbb{R}^{n \times 1} \) to the input dataset \( X \) consists of corresponding \( n \) class labels. Let each record \( x[i] \) has an observation result \( y[i] \) with \( c \) possible classes labelled as \( y_i \in \{0, 1, \ldots, c - 1\} \). The multiclass logistic regression model has \( c \) parameter vectors \( w_i \) of size \((1 + d)\), which form the parameter matrix \( W \). Each vector \( w_i \) is used to model the probability of each class label.
with the label class \( y \) where

For simplicity in presentation, we first consider the case of dataset \( X \) or its log-likelihood function

and probability. Each class label for each record by the softmax function and output the class label with the maximum

MLR aims to find the best parameter matrix \( W \) such that the algorithm can model the probabilities of each class label for each record by the softmax function and output the class label with the maximum probability.

\[
P = \begin{bmatrix}
    p[1][0] & p[1][1] & \cdots & p[1][c-1] \\
    p[2][0] & p[2][1] & \cdots & p[2][c-1] \\
    \vdots & \vdots & \ddots & \vdots \\
    p[n][0] & p[n][1] & \cdots & p[n][c-1]
\end{bmatrix}
\]

\[= \begin{bmatrix}
    \text{Prob}(y = 0|x = x_1) & \text{Prob}(y = 1|x = x_1) & \cdots & \text{Prob}(y = c - 1|x = x_1) \\
    \text{Prob}(y = 0|x = x_2) & \text{Prob}(y = 1|x = x_2) & \cdots & \text{Prob}(y = c - 1|x = x_2) \\
    \vdots & \vdots & \ddots & \vdots \\
    \text{Prob}(y = 0|x = x_n) & \text{Prob}(y = 1|x = x_n) & \cdots & \text{Prob}(y = c - 1|x = x_n)
\end{bmatrix},
\]

where

\[p_{i|j} = \text{Prob}(y = j|x = x_i) = \frac{\exp(x_i \cdot w_j^T)}{\sum_{k=0}^{c-1} \exp(x_i \cdot w_k^T)}\]

and

\[\sum_{j=0}^{c-1} p_{i|j} = \text{Prob}(y = 0|x = x_i) + \cdots + \text{Prob}(y = c - 1|x = x_i) = 1 \text{ for } 1 \leq i \leq n.\]

Multiclass LR is to maximize

\[L = \prod_{i=1}^{n} \text{Prob}(y = y_i|x = x_i) = \prod_{i=1}^{n} \frac{\exp(x_i \cdot w_{y_i}^T)}{\sum_{k=0}^{c-1} \exp(x_i \cdot w_k^T)}\]

or its log-likelihood function

\[\ln L = \sum_{i=1}^{n} \left[ x_i \cdot w_{y_i}^T - \ln \sum_{k=0}^{c-1} \exp(x_i \cdot w_k^T) \right].\]

For simplicity in presentation, we first consider the case of dataset \( X \) consisting of just one sample \( x_1 \) with the label class \( y_1 \).

\[
\frac{\partial \ln L}{\partial w_k (k = y_1)} = x_1 \cdot 1 - \frac{x_1 \cdot \exp(x_1 \cdot w_{y_1}^T)}{\sum_{k=0}^{c-1} \exp(x_1 \cdot w_k^T)} = x_1 \cdot [1 - \text{Prob}(y = y_1|x = x_1)]
\]

(1)

\[
\frac{\partial \ln L}{\partial w_k (k \neq y_1)} = x_1 \cdot 0 - \frac{x_1 \cdot \exp(x_1 \cdot w_{y_1}^T)}{\sum_{k=0}^{c-1} \exp(x_1 \cdot w_k^T)} = x_1 \cdot [0 - \text{Prob}(y = y_1|x = x_1)]
\]

(2)
Here comes the one-hot encoding method with its practical use in uniting formulas [1] and [2].

One-hot encoding is the most widely adopted technique of representing categorical data as a binary vector. For a class label \( y_i \) with \( c \) possible values, one-hot encoding converts \( y_i \) into a vector \( \vec{y}_i \) of size \( c \) such that \( \vec{y}_i[j] = 1 \) if \( j = y_i \) and \( \vec{y}_i[j] = 0 \) otherwise: \( \vec{y}_i \overset{\text{one-hot encoding}}{\mapsto} \vec{y}_i = [y_i[0]; y_i[1]; \ldots; y_i[c-1]] \). Therefore, the outcome \( \bar{Y} \in \mathbb{N}^{n \times c} \) can be transformed by this encoding method into \( Y \in \mathbb{N}^{n \times 1} \):

\[
Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \overset{\text{one-hot encoding}}{\mapsto} \bar{Y} = \begin{bmatrix} [y_1[1] & \cdots & y_1[c-1]] \\ [y_2[1] & \cdots & y_2[c-1]] \\ \vdots \\ [y_n[1] & \cdots & y_n[c-1]] \end{bmatrix}.
\]

We can hence obtain a single unified formula with the help of the one-hot encoding of \( y_i \):

\[
\frac{\partial \log \text{likelihood}}{\partial w_k} = y_i[k] \cdot x_1 - \frac{x_1 \cdot \exp(x_1 \cdot w_i)}{\sum_{k=0}^{c-1} \exp(x_1 \cdot w_k)} = x_1 \cdot [y_i[k] - \text{Prob}(y = y_i|x = x_1)],
\]

which yields the gradient of \( \ln L \):

\[
\nabla = \frac{\partial \ln L}{\partial \pi} = \left[ \frac{\partial \ln L}{\partial w_0}, \frac{\partial \ln L}{\partial w_1}, \ldots, \frac{\partial \ln L}{\partial w_{c-1}} \right]^T = \left[ \frac{\partial \ln L}{\partial w_0}, \frac{\partial \ln L}{\partial w_1}, \ldots, \frac{\partial \ln L}{\partial w_{c-1}} \right]^T = [x_1 \cdot [\vec{y}_i[0] - p_{i[0]}], x_1 \cdot [\vec{y}_i[1] - p_{i[1]}], \ldots, x_1 \cdot [\vec{y}_i[c-1] - p_{i[c-1]}]]
\]

or could be reshaped to the same dimension as \( W \):

\[
\nabla = [\vec{y}_i - p_i]^T \cdot x_1
\]

for the convenience in gradient computation: \( W = W + [\nabla] \).

The log-likelihood \( \ln L \) should be seen as a multivariate function of \([(1 + c)(1 + d)] \) variables, whose gradient is a column vector of size \([(1 + c)(1 + d)] \) and whose Hessian matrix \( \nabla^2 \) is literally a square matrix of order \([(1 + c)(1 + d)] \).

\[
\nabla^2 = \begin{bmatrix}
\frac{\partial^2 \ln L}{\partial w_0^2} & \cdots & \frac{\partial^2 \ln L}{\partial w_0 \partial w_{c-1}} \\
\frac{\partial^2 \ln L}{\partial w_1 \partial w_0} & \cdots & \frac{\partial^2 \ln L}{\partial w_1 \partial w_{c-1}} \\
\vdots & \ddots & \vdots \\
\frac{\partial^2 \ln L}{\partial w_{c-1} \partial w_0} & \cdots & \frac{\partial^2 \ln L}{\partial w_{c-1} \partial w_{c-1}}
\end{bmatrix} = \begin{bmatrix}
[p_0[0] \cdot (p_0[0] - 1)] \cdot x_1^T \cdot x_1 & \cdots & [p_0[0] \cdot p_0[c-1] \cdot x_1^T \cdot x_1] \\
[p_1[0] \cdot p_0[0] \cdot x_1^T \cdot x_1] & \cdots & [p_1[0] \cdot p_0[c-1] \cdot x_1^T \cdot x_1] \\
\vdots & \ddots & \vdots \\
[p_{c-1}[0] \cdot x_1^T \cdot x_1] & \cdots & [p_{c-1}[c-1] \cdot (p_{c-1}[c-1] - 1)] \cdot x_1^T \cdot x_1 \end{bmatrix} \\
\otimes [x_1^T \cdot x_1],
\end{bmatrix}
\]

where \( \frac{\partial^2 \ln L}{\partial w_k \partial w_l} = \frac{\partial^2 \ln L}{\partial w_l \partial w_k} = [p_k[i] \cdot (p_k[i] - 1)] \cdot x_l^T \cdot x_k \) for \( i = j \) and \( \frac{\partial^2 \ln L}{\partial w_k \partial w_k} = [p_k[i] \cdot (p_k[i] - 0)] \cdot x_k^T \cdot x_k \) for \( i \neq j \) and “\( \otimes \)” is the Kronecker product.

Kronecker product, unlike the usual matrix multiplication, is an operation that is performed on two matrices of arbitrary size to result in a block matrix. For an \( m \times n \) matrix \( A \) and a \( p \times q \) matrix \( B \),
the kronecker product of $A$ and $B$ is a $pm \times qn$ block matrix, denoted by $A \otimes B$:

$$A \otimes B = \begin{bmatrix}
  a_{11}B & a_{12}B & \cdots & a_{1n}B \\
  a_{21}B & a_{22}B & \cdots & a_{2n}B \\
  \vdots & \vdots & \ddots & \vdots \\
  a_{m1}B & a_{m2}B & \cdots & a_{mn}B \\
\end{bmatrix}$$

where $a_{ij}$ and $b_{kl}$ are the elements of $A$ and $B$ respectively.

The inverse of the kronecker product $A \otimes B$ exists if and only if $A$ and $B$ are both invertable, and can be obtained by

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}. \tag{3}$$

This invertible product property can be used to facilitate the calculation of the inverse $[\frac{\partial^2 \ln L}{\partial \pi \partial \pi}]^{-1}$ of Hessian matrix $\nabla^2$:

$$[\frac{\partial^2 \ln L}{\partial \pi \partial \pi}]^{-1} = \begin{bmatrix}
  p[1][0](p[1][0] - 1) & p[1][0]p[1][1] & \cdots & p[1][0]p[1][c-1] \\
  p[1][1]p[1][0] & p[1][1]p[1][1] - 1 & \cdots & p[1][1]p[1][c-1] \\
  \vdots & \vdots & \ddots & \vdots \\
  p[1][c-1]p[1][0] & p[1][c-1]p[1][1] & \cdots & p[1][c-1](p[1][c-1] - 1) \\
\end{bmatrix}^{-1} \otimes [x_1^T x_1]^{-1}. \tag{4}$$

Böhning [2] presented another lemma about kronecker product: If $A \leq B$ in the Loewner order then $A \otimes C \leq B \otimes C$.

To apply the quadratic gradient in the multiclass LR, we need to build the matrix $\bar{B}$ first, trying to find a fixed Hessian matrix. We could try to build it directly from the Hessian matrix $\nabla^2$ based on the construction method of quadratic gradient:

$$\bar{B} = \begin{bmatrix}
  \bar{B}_{[0]} & 0 & \cdots & 0 \\
  0 & \bar{B}_{[1]} & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & \bar{B}_{[c-1]} \\
\end{bmatrix} = \text{diag}\{\bar{B}_{[0][0]}, \bar{B}_{[0][1]}, \cdots, \bar{B}_{[0][d]}, \bar{B}_{[1][0]}, \bar{B}_{[1][1]}, \cdots, \bar{B}_{[1][d]}, \cdots, \bar{B}_{[c-1][0]}, \bar{B}_{[c-1][1]}, \cdots, \bar{B}_{[c-1][d]}\},$$

where $\bar{B}_{[i][j]} = |p[i][j]p[i][0]| + |p[i][j]p[i][1]| + \cdots + |p[i][j](p[i][j] - 1)| + |p[i][j]p[i][j+1]| + \cdots + |p[i][j]p[i][c-1]| \times (|x_{i}[j][x_{i}[1][0]| + \cdots + |x_{i}[j][x_{i}[1][d]|) + \varepsilon.$

Since $0 < p[i][j] < 1$ and $\sum_{j=0}^{c-1} p[i][j] = \text{Prob}(y = 0|x = x_i) + \cdots + \text{Prob}(y = c-1|x = x_i) = 1$ for $1 \leq i \leq n$, we get:

$$\bar{B}_{[i][j]} = |p[i][j]p[i][0]| + |p[i][j]p[i][1]| + \cdots + |p[i][j](p[i][j] - 1)|$$

$$= |p[i][j]|p[i][0]| + |p[i][j]p[i][1]| + \cdots + |p[i][j](1 - p[i][j])|$$

$$= 2 \cdot p[i][j](1 - p[i][j]) \times (|x_{i}[j][x_{i}[1][0]| + \cdots + |x_{i}[j][x_{i}[1][d]|) + \varepsilon$$

$$\leq 0.5 \times (|x_{i}[j][x_{i}[1][0]| + \cdots + |x_{i}[j][x_{i}[1][d]|) + \varepsilon.$$
The dataset $X$ should be normalized into the range $[0, 1]$ in advance, further leading $\bar{B}_{ij}$ to:

$$\bar{B}_{ij} \leq 0.5 \times (x_{i[0]}x_{j[0]} + \ldots + x_{i[q]}x_{j[d]}) + \varepsilon.$$  

It is straightforward to verify that setting $B_{ij} = 0.5 \times (x_{i[0]}x_{j[0]} + \ldots + x_{i[q]}x_{j[d]}) + \varepsilon$ also meets the convergence condition of fixed Hessian Newton’s method, in which case $\bar{B}$ could be built directly from $\bar{H} = \frac{1}{2} E \otimes x_1^T x_1$.

For the common cases where the dataset $X$ is a sample of size $n$:

$$\nabla = \sum_{i=1}^{n} [\bar{y}_i] - p[i] \cdot x[i] = [\bar{Y} - P] \cdot X,$$

$$\frac{\partial^2 \ln L}{\partial \pi \partial \pi} = \sum_{i=1}^{n} \begin{bmatrix} p[i][0] & p[i][0] - 1 & \cdots & p[i][c[i] - 1] \\ p[i][1] & p[i][1] - 1 & \cdots & p[i][c[i] - 1] \\ \vdots & \vdots & \ddots & \vdots \\ p[i][c - 1] & p[i][c - 1] & \cdots & p[i][c - 1] - 1 \end{bmatrix} \otimes [x_i^T x_i] = [P^T P - \text{diag}\{\sum_{i=1}^{n} p[i][0], \ldots, \sum_{i=1}^{n} p[i][d]\}] \otimes [X^T X].$$

With the lemma[3] and other kronecker product properties we could conclude:

$$\bar{B}_{ij} \leq \sum_{i=1}^{n} 0.5 \times (x_{i[0]}x_{j[0]} + \ldots + x_{i[q]}x_{j[d]}) + \varepsilon$$

$$\leq 0.5 \times \sum_{i=1}^{n} (x_{i[0]}x_{j[0]} + \ldots + x_{i[q]}x_{j[d]}) + \varepsilon.$$  

That is, $\bar{B}$ can also be built from $\bar{H} = \frac{1}{2} E \otimes X^T X$ and Böhning and Lindsay[3] gave the same matrix as a good lower bound for cox proportional hazards model. We thus obtain the quadratic gradient $G = \bar{B}^{-1} \times \nabla$ and the iteration formula of the naive quadratic gradient ascent method in vector form:

$$\pi^T = \pi^T + G$$  

or in matrix form: $W = W + MG$ where $MG_{[i,j]} = \bar{B}_{ij(i+d)+j}$.  

Algorithm 1 and Algorithm 2 describe the enhanced NAG method and the enhanced Adagrad algorithm via quadratic gradient respectively.

## 4 Experiments

All the python source code to implement the experiments in the paper is openly available at: [https://github.com/petitioner/ML.MulticlassLRtraining](https://github.com/petitioner/ML.MulticlassLRtraining).

To study the performance of the enhanced NAG and Adagrad methods for multiclass LR, we consider three datasets adopted by [1]: vehicle, shuttle, and segmentation taken from LIBSVM Data. Table 1 describes the three datasets. We also used the testing data of the shuttle dataset in the training stage. Maximum likelihood estimation (the loss function) and accuracy are selected as the only indicators. We compare the performance of the enhanced methods with their corresponding first-order naive gradient method. The accuracy and maximum likelihood estimation are reported in Figures 3 and 4.

We can remark that the performances of the enhanced methods outperform their original ones.

### Table 1: Characteristics of the several datasets used in our experiments

| Dataset | No. Samples (training) | No. Samples (testing) | No. Features | No. Classes |
|---------|-------------------------|-----------------------|--------------|-------------|
| iris    | 150                     | N/A                   | 4            | 3           |
| segment | 2,310                   | N/A                   | 19           | 7           |
| shuttle | 43,500                  | 14,500                | 9            | 7           |
| vehicle | 846                     | N/A                   | 18           | 4           |

[https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/multiclass.html](https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/multiclass.html)
5 Conclusion

There is a good chance that the enhanced gradient methods for multiclass LR could be used in the classification neural-network training via the softmax activation and the cross-entropy loss.

References

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Figure 1: Training results PREC for SFHNewton vs. Adagrad vs. Enhanced Adagrad

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Figure 2: Training results LOSS for SFHNewton vs. Adagrad vs. Enhanced Adagrad
Algorithm 2 The enhanced Adaptive Gradient Algorithm for Multiclass LR Training

**Input:** training dataset $X \in \mathbb{R}^{n \times (1+d)}$; one-hot encoding training label $Y \in \mathbb{R}^{n \times c}$; and the number $\kappa$ of iterations;

**Output:** the parameter matrix $V \in \mathbb{R}^{c \times (1+d)}$ of the multiclass LR

1: Set $H \leftarrow -\frac{1}{H}X^TX$ \hfill \triangleright \: H \in \mathbb{R}^{(1+d) \times (1+d)}
2: Set $W \leftarrow 0$, $B \leftarrow 0$ \hfill \triangleright \: W \in \mathbb{R}^{c \times (1+d)}$, $B \in \mathbb{R}^{c \times (1+d)}
3: for $j := 0$ to $d$ do
4: \hspace{1em} $B[0][j] \leftarrow \varepsilon$ \hfill \triangleright \: \varepsilon$ is a small positive constant such as $1e-8$
5: \hspace{1em} for $i := 0$ to $d$ do
6: \hspace{2em} $B[0][j] \leftarrow B[0][j] + |H[i][j]|$
7: \hspace{1em} end for
8: \hspace{1em} end for
9: \hspace{1em} for $i := 1$ to $c-1$ do
10: \hspace{2em} $B[i][j] \leftarrow B[0][j]$
11: \hspace{1em} end for
12: \hspace{1em} for $i := 0$ to $c-1$ do
13: \hspace{2em} $B[i][j] \leftarrow 1.0/B[i][j]$
14: \hspace{1em} end for
15: \hspace{1em} end for
16: Set $Gt \leftarrow 0$ \hfill \triangleright \: Gt \in \mathbb{R}^{c \times (1+d)}$
17: Set $\alpha_0 \leftarrow 0.01$, $\alpha_1 \leftarrow 0.5 \times (1 + \sqrt{1 + 4 \times \alpha_0^2})$
18: for $\text{count} := 1$ to $\kappa$ do
19: \hspace{1em} Set $Z \leftarrow X \times W^T$ \hfill \triangleright \: Z \in \mathbb{R}^{n \times c}$ and $W^T$ means the transpose of matrix $W$
20: \hspace{1em} for $i := 1$ to $n$ do \hfill \triangleright \: Z is going to store the inputs to the softmax function
21: \hspace{2em} Set $\text{rowsum} \leftarrow 0$
22: \hspace{2em} for $j := 0$ to $d$ do
23: \hspace{3em} $Z[i][j] \leftarrow e^{Z[i][j]}$ \hfill \triangleright \: $e^{Z[i][j]}$ is to compute $\exp\{Z[i][j]\}$
24: \hspace{3em} $\text{rowsum} \leftarrow \text{rowsum} + Z[i][j]$
25: \hspace{2em} end for
26: \hspace{1em} end for
27: $Z[i][j] \leftarrow Z[i][j]/\text{rowsum}$ \hfill \triangleright \: Z now stores the outputs of the softmax function
28: \hspace{1em} end for
29: Set $g \leftarrow (Y - Z)^T \times X$ \hfill \triangleright \: g \in \mathbb{R}^{c \times (1+d)}$
30: Set $G \leftarrow 0$
31: for $i := 0$ to $c-1$ do
32: \hspace{1em} for $j := 0$ to $d$ do
33: \hspace{2em} $G[i][j] \leftarrow B[i][j] \times g[i][j]$
34: \hspace{2em} end for
35: \hspace{1em} end for
36: \hspace{1em} end for
37: \hspace{1em} for $i := 0$ to $c-1$ do
38: \hspace{2em} for $j := 0$ to $d$ do
39: \hspace{3em} $Gt[i][j] \leftarrow Gt[i][j] + G[i][j] \times G[i][j]$
40: \hspace{3em} end for
41: \hspace{2em} end for
42: \hspace{1em} end for
43: \hspace{1em} end for
44: Set $\Gamma \leftarrow 0$ \hfill \triangleright \: $\Gamma \in \mathbb{R}^{c \times (1+d)}$
45: for $i := 0$ to $c-1$ do
46: \hspace{1em} for $j := 0$ to $d$ do
47: \hspace{2em} $\Gamma[i][j] \leftarrow (1.0 + 0.01)/\sqrt{\varepsilon + Gt[i][j]}$
48: \hspace{2em} end for
49: \hspace{1em} end for
50: \hspace{1em} $W[i][j] \leftarrow W[i][j] + \Gamma[i][j] \times G[i][j]$
51: \hspace{1em} end for
52: \hspace{1em} end for
53: return $W$
Figure 3: Training results PREC for SFHNewton vs. Adagrad vs. Enhanced Adagrad
Figure 4: Training results LOSS for SFHNewton vs. NAG vs. NAGG