Proximal Quasi-Newton for Computationally Intensive
\(\ell_1\)-regularized \(M\)-estimators

Kai Zhong ∗ Ian E.H. Yen † Inderjit S. Dhillon † Pradeep Ravikumar †
July 1, 2014

Abstract

We consider the class of optimization problems arising from computationally intensive \(\ell_1\)-regularized \(M\)-estimators, where the function or gradient values are very expensive to compute. A particular instance of interest is the \(\ell_1\)-regularized MLE for learning Conditional Random Fields (CRFs), which are a popular class of statistical models for varied structured prediction problems such as sequence labelling, alignment, and classification with label taxonomy. \(\ell_1\)-regularized MLEs for CRFs are particularly expensive to optimize since computing the gradient values requires an expensive inference step. In this work, we propose the use of a carefully constructed proximal quasi-Newton algorithm for such computationally intensive \(M\)-estimation problems, where we employ an aggressive active set selection technique. In a key contribution of the paper, we show that the proximal quasi-Newton method is provably \textit{super-linearly convergent}, even in the absence of strong convexity, by leveraging a restricted variant of strong convexity. In our experiments, the proposed algorithm converges considerably faster than current state-of-the-art on the problems of sequence labeling and hierarchical classification.

1 Introduction

\(\ell_1\)-regularized \(M\)-estimators have attracted considerable interest in recent years due to their ability to fit large-scale statistical models, where the underlying model parameters are sparse. The optimization problem underlying these \(\ell_1\)-regularized \(M\)-estimators takes the form:

\[
\min_w f(w) := \lambda\|w\|_1 + \ell(w),
\]

where \(\ell(w)\) is a convex differentiable loss function. In this paper, we are particularly interested in the case where the function or gradient values are very expensive to compute; we refer to these functions as computationally intensive functions, or CI functions in short. A particular case of interest are \(\ell_1\)-regularized MLEs for Conditional Random Fields (CRFs), where computing the gradient requires an expensive inference step.

There has been a line of recent work on computationally efficient methods for solving (1), including [2, 8, 13, 21, 23, 4]. It has now become well understood that it is key to leverage the sparsity of the optimal solution by maintaining sparse intermediate iterates [2, 5, 8]. Coordinate Descent (CD) based methods, like CDN [8], maintain the sparsity of intermediate iterates by focusing on an active set of working variables. A caveat with such methods is that, for CI function, each coordinate update typically requires a call of inference oracle to evaluate partial derivative for single coordinate. One approach adopted in [16] to address this is using Blockwise Coordinate Descent that updates a block of variables at a time by ignoring the second-order effect, which however sacrifices the convergence guarantee. Newton-type methods have also attracted a surge of interest in recent years [5, 13], but these require computing the exact Hessian or Hessian-vector product, which is very expensive for CI functions. This then suggests the use of quasi-Newton methods, popular instances of which include OWL-QN [23], which is adapted from \(\ell_2\)-regularized L-BFGS, as well as Projected Quasi-Newton (PQN) [4]. A key caveat with OWL-QN and PQN however is that they do not exploit the sparsity of the underlying solution. In this paper, we consider the class of \textit{Proximal Quasi-Newton} (Prox-QN) methods, which we argue seem particularly well-suited to such CI functions, for the following three reasons. Firstly, it requires gradient evaluations only once in each outer iteration. Secondly, it is a second-order method, which has asymptotic superlinear convergence. Thirdly, it can

* Institute for Computational Engineering and Science, University of Texas at Austin, zhongkai@ices.utexas.edu
† Computer Science, University of Texas at Austin, {ianyen, inderjit, pradeepr}@cs.utexas.edu
employ some active-set strategy to reduce the time complexity from $O(d)$ to $O(nnz)$, where $d$ is the number of parameters and $nnz$ is the number of nonzero parameters.

While there has been some recent work on Prox-QN algorithms [2, 3], we carefully construct an implementation that is particularly suited to CI $\ell_1$-regularized $M$-estimators. We carefully maintain the sparsity of intermediate iterates, and at the same time reduce the gradient evaluation time. A key facet of our approach is our aggressive active set selection (which we also term a ”shrinking strategy”) to reduce the number of active variables under consideration at any step, and correspondingly the number of evaluations of partial gradients in each iteration. Our strategy is particularly aggressive in that it runs over multiple epochs, and in each epoch, chooses the next working set as a subset of the current working set rather than the whole set; while at the end of an epoch, allows for other variables to come in. As a result, in most iterations, our aggressive shrinking strategy only requires the evaluation of partial gradients in the current working set. Moreover, we adapt the L-BFGS update to the shrinking procedure such that the update can be conducted without any loss of accuracy caused by aggressive shrinking.

Thirdly, we store our data in a feature-indexed structure to combine data sparsity as well as iterate sparsity. We carefully maintain the sparsity of intermediate estimators.

To summarize, our contributions are twofold. (a) We present a carefully constructed proximal quasi-Newton method for computationally intensive (CI) $\ell_1$-regularized $M$-estimators, which we empirically show to outperform many state-of-the-art methods on CRF problems. (b) We provide the first proof of asymptotic superlinear convergence for Prox-QN method without strong convexity, but under a restricted variant of strong convexity, termed Constant Nullspace Strong Convexity (CNSC), which is typically satisfied by standard $M$-estimators, including the $\ell_1$-regularized CRF MLEs.

## 2 Proximal Quasi-Newton Method

A proximal quasi-Newton approach to solve $M$-estimators of the form [1] proceeds by iteratively constructing a quadratic approximation of the objective function [1] to find the quasi-Newton direction, and then conducting a line search procedure to obtain the next iterate.

Given a solution estimate $w_t$ at iteration $t$, the proximal quasi-Newton method computes a descent direction by minimizing the following regularized quadratic model,

$$d_t = \arg \min_{\Delta} g_t^T \Delta + \frac{1}{2} \Delta^T B_t \Delta + \lambda \|w_t + \Delta\|_1$$  \hspace{1cm} (2)

where $g_t = g(w_t)$ is the current gradient and $B_t$ is an approximation to the Hessian of $\ell(w)$. $B_t$ is usually formulated by the L-BFGS algorithm. This subproblem [2] can be efficiently solved by randomized coordinate descent algorithm as shown in section 2.2.

The next iterate is obtained from the backtracking line search procedure, $w_{t+1} = w_t + \alpha_t d_t$, where the step size $\alpha_t$ is tried over $\{\beta^0, \beta^1, \beta^2, ...\}$ until the Armijo rule is satisfied,

$$f(w_t + \alpha d_t) \leq f(w_t) + \alpha \sigma \Delta_t,$$

where $0 < \beta < 1$, $0 < \sigma < 1$ and $\Delta_t = g_t^T d_t + \lambda (\|w_t + d_t\|_1 - \|w_t\|_1)$.

### 2.1 BFGS update formula

$B_t$ can be updated by the gradients of the previous iterations according to the BFGS update [18].

$$B_t = B_{t-1} - \frac{B_{t-1} s_{t-1} s_{t-1}^T B_{t-1}}{s_{t-1}^T B_{t-1} s_{t-1}} + \frac{y_{t-1} y_{t-1}^T}{y_{t-1}^T s_{t-1}}$$  \hspace{1cm} (3)

where $s_t = w_{t+1} - w_t$ and $y_t = g_{t+1} - g_t$.

We use the compact formula for $B_t$ [18].

$$B_t = B_0 - QRQ^T = B_0 - Q\hat{Q},$$

2
Since we only update the coordinates in the working set, the above algorithm has only computation complexity $O(|A|)$ where $A$ is the $j$-th column of $d$. For experiments show that the number of epochs is typically between 3-5. Fortunately, our approach is that at the first iteration of each new epoch, the entire gradient over all coordinates is evaluated, the computation time for those iterations accounts for a significant portion of the total time complexity. Fortunately, our experiments show that the number of epochs is typically between 3-5.

\[ Q := \begin{bmatrix} B_0 S_t & Y_t \end{bmatrix}, \quad R := \begin{bmatrix} S_t^T B_0 S_t & L_t \cr L_t^T & -D_t \end{bmatrix}^{-1}, \quad \hat{Q} := RQ^T \]

\[ S_t = [s_0, s_1, \ldots, s_{t-1}], \quad Y_t = [y_0, y_1, \ldots, y_{t-1}] \]

\[ D_t = \text{diag}[s_0^T y_0, \ldots, s_{t-1}^T y_{t-1}] \quad \text{and} \quad (L_t)_{i,j} = \begin{cases} s_{i-1}^T y_{j-1} & \text{if } i > j \\ 0 & \text{otherwise} \end{cases} \]

In practical implementation, we apply Limited-memory-BFGS. It only uses the information of the most recent $m$ gradients, so that $Q$ and $\hat{Q}$ have only size, $d \times 2m$ and $2m \times d$, respectively. $B_t$ is usually set as $\gamma_t I$ for computing $B_t$, where $\gamma_t = y_{t-1}^T s_{t-1}/s_{t-1}^T s_{t-1}$ [13]. As will be discussed in section 2.3, $Q(\hat{Q})$ is updated just on the rows(columns) corresponding to the working set, $A$. We have the time complexity for L-BFGS update, $O(m^2|A| + m^3)$.

### 2.2 Coordinate Descent for Inner Problem

Randomized coordinate descent is carefully employed to solve the inner problem (2) by Tang and Scheinberg [2].

In the update for coordinate $j$, $d \leftarrow d + z^* e_j$, $z^*$ is obtained by solving the one-dimension problem,

\[ z^* = \arg \min_z \frac{1}{2} (B_t)_{jj} z^2 + (d_j) z + \lambda \|w_t\|d_j + d_j + z \]

This one-dimension problem has a closed-form solution

\[ z^* = -c + S(c - b/a, \lambda/a) \quad (4) \]

where $S$ is the soft-threshold function and $a = (B_t)_{jj}$, $b = (g_t)_j + (B_t d)_j$ and $c = (w_t)_j + d_j$.

For $B_0 = \gamma_t I$, the diagonal of $B_t$ can be computed by $(B_t)_{jj} = \gamma_t - q_j^T q_j$, where $q_j^T$ is the $j$-th column of $Q$. And the second term in $b$, $(B_t d)_j$ can be computed by,

\[ (B_t d)_j = \gamma_t d_j - q_j^T \hat{Q} d = \gamma_t d_j - q_j^T d, \]

where $\hat{d} = \hat{Q} d$. Since $\hat{d}$ has only $2m$ dimension, it is fast to update $(B_t d)_j$ by $q_j$ and $\hat{d}$. In each inner iteration, only $d_j$ is updated, so we have the fast update of $\hat{d}$, $\hat{d} \leftarrow \hat{d} + q_j z^*$.

Since we only update the coordinates in the working set, the above algorithm has only computation complexity $O(m|A| \times \text{inner iter})$, where $\text{inner iter}$ is the number of iterations used for solving the inner problem.

### 2.3 Implementation

In this section, we discuss several key implementation details used in our algorithm to speed up the optimization.

#### Shrinking Strategy

In each iteration, we select an active or working subset $A$ of the set of all variables: only the variables in this set are updated in the current iteration. The complementary set, also called the fixed set, is set to zero and is not updated. The use of such a shrinking strategy reduces the overall complexity from $O(d)$ to $O(|A|)$. Specifically, we (a) update the gradients just on the working set, (b) update $Q(\hat{Q})$ just on the rows(columns) corresponding to the working set, and (c) compute the latest entries in $D_t$, $\gamma_t$, $L_t$ and matrix $S_t^T S_t$ by just using the corresponding working set rather than the whole set.

The key facet of our “shrinking strategy” however is in aggressively shrinking the active set: at the next step, we set the active set to be a subset of the previous active set, so that $A_t \subset A_{t-1}$. Such an aggressive shrinking strategy however is not guaranteed to only weed out irrelevant variables. Accordingly, we proceed in epochs. In each epoch, we progressively shrink the active set as above, till the iterations seem to converge. At that time, we then allow for all the “shrunk” variables to come back and start a new epoch. Such a strategy was also called an $\epsilon$-cooling strategy by Fan et al. [14], where the shrinking stopping criterion is loose at the beginning, and progressively becomes more strict each time all the variables are brought back. For L-BFGS update, when a new epoch starts, the memory of L-BFGS is cleaned to prevent any loss of accuracy.

Because at the first iteration of each new epoch, the entire gradient over all coordinates is evaluated, the computation time for those iterations accounts for a significant portion of the total time complexity. Fortunately, our experiments show that the number of epochs is typically between 3-5.
Inexact inner problem solution
Like many other proximal methods, e.g. GLMNET and QUIC, we solve the inner problem inexactly. This reduces the time complexity of the inner problem dramatically. The amount of inexactness is based on a heuristic method which aims to balance the computation time of the inner problem in each outer iteration. The computation time of inner problem is determined by the number of inner iterations and the size of working set. Thus, we let the number of inner iterations, \(n_{\text{inner}} = \min\{\max_{\text{inner}}, \lfloor d/|A| \rfloor\}\), where \(\max_{\text{inner}} = 10\) in our experiment.

Data Structure for both model sparsity and data sparsity
In our implementation we take two sparsity patterns into consideration: (a) model sparsity, which accounts for the fact that most parameters are equal to zero in the optimal solution; and (b) data sparsity, wherein most feature values of any particular instance are zeros. We use a feature-indexed data structure to take advantage of both sparsity patterns. Computations involving data will be time-consuming if we compute over all the instances including those that are zero. So we leverage the sparsity of data in our experiment by using vectors of pairs, whose members are the index and its value. Traditionally, each vector represents an instance and the indices in its pairs are the feature indices. However, in our implementation, to take both model sparsity and data sparsity into account, we use an inverted data structure, where each vector represents one feature (feature-indexed) and the indices in its pairs are the instance indices. This data structure facilitates the computation of the gradient for a particular feature, which involves only the instances related to this feature.

We summarize these steps in the algorithm below.

Algorithm 1 Proximal Quasi-Newton Algorithm

Input: Dataset \(\{x^{(i)}, y^{(i)}\}_{i=1,2,...,N}\), termination criterion \(\epsilon\) and L-BFGS memory size \(m\).

Output: \(w^*\) converging to arg min\(_w f(w)\).

1: Initialize \(w \leftarrow 0, g \leftarrow \partial \phi/\partial w\), working set \(A \leftarrow \{1, 2, \ldots, d\}\), and \(S, Y, Q, \hat{Q} \leftarrow \phi\).
2: while termination criterion is not satisfied or working set doesn’t contain all the variables do
3: Shrinking working set.
4: if Shrinking stopping criterion is satisfied then
5: Take all the shrunken variables back to working set and clean the memory of L-BFGS.
6: Update Shrinking stopping criterion and continue.
7: end if
8: Solve inner problem \(2\) over working set and obtain the new direction \(d\).
9: Conduct line search based on Armijo rule and obtain new iterate \(w\).
10: Update \(g, s, y, S, Y, Q, \hat{Q}\) and related matrices over working set.
11: end while

3 Convergence Analysis

In this section, we analyze the convergence behavior of proximal quasi-Newton method. In current literature, the analysis of proximal Newton-type methods relies on the assumption of strongly convex objective function to prove superlinear convergence [3]; otherwise, only sublinear rate can be proved [25]. However, our objective \(\phi\) is not strongly convex when the dimension is very large or there are redundant features. In particular, the Hessian matrix \(H(w)\) of the smooth function \(\ell(w)\) is not positive-definite. We thus leverage a recently introduced restricted variant of strong convexity, termed Constant Nullspace Strong Convexity (CNSC) in [11]. There the authors analyzed the behavior of proximal gradient and proximal Newton methods under such a condition. The proximal quasi-Newton procedure in this paper however requires a subtler analysis, but in a key contribution of the paper, we are nonetheless able to show asymptotic superlinear convergence of the Prox-QN method under this restricted variant of strong convexity.

Definition 1 (Constant Nullspace Strong Convexity (CNSC)). A composite function \(\phi\) is said to have Constant Nullspace Strong Convexity restricted to space \(\mathcal{T}\) (CNSC-\(\mathcal{T}\)) if there is a constant vector space \(\mathcal{T}\) s.t. \(\ell(w)\) depends only on \(z = \text{proj}_\mathcal{T}(w)\), i.e. \(\ell(w) = \ell(z)\), and its Hessian satisfies

\[
m\|v\|^2 \leq v^T H(w) v \leq M \|v\|^2, \quad \forall v \in \mathcal{T}, \forall w \in \mathbb{R}^d
\]

for some \(M \geq m > 0\), and

\[
H(w) v = 0, \quad \forall v \in \mathcal{T}^\perp, \forall w \in \mathbb{R}^d,
\]
where $\mathcal{T}^\perp$ is the complementary space orthogonal to $\mathcal{T}$.

This condition can be seen to be an algebraic condition that is satisfied by typical $M$-estimators considered in high-dimensional settings. We use $\text{proj}_T(w)$ to denote the projection of $w$ onto $\mathcal{T}$. Let $\text{proj}_T(w) = UU^T w$, where $U \in \mathbb{R}^{d \times d}$, $d \leq d$ is the dimension of $\mathcal{T}$ space, and $U^T U = I$.

**Theorem 1** (Asymptotic Superlinear Convergence). For $B_1$ and the Lipchitz-continuous $\nabla^2 \ell(w)$ satisfying CNSC-$\mathcal{T}$ condition, the proximal quasi-Newton update has $q$-superlinear convergence:

$$
\|z_{t+1} - z^*\| \leq o(\|z_t - z^*\|),
$$

where $z_t = U^T w_t$, $z^* = U^T w^*$ and $w^*$ is an optimal solution of (1).

The proof is given in Appendix 7.1. We prove it by exploiting the CNSC-$\mathcal{T}$ property. First, we re-build our problem and algorithm on the reduced space $Z = \{z \in \mathbb{R}^d | z = U^T w\}$, where the strong-convexity property holds. Then we prove the asymptotic superlinear convergence on $Z$ following Theorem 3.7 in [26].

**Theorem 2.** The sequence $\{w_t\}_{t=1}^\infty$ produced by the proximal quasi-Newton Method has

$$
f(w_t) - f(w^*) \leq L \|z_t - z^*\|,
$$

where $L = L_\ell + \lambda \sqrt{d}$, $L_\ell$ is the Lipchitz-continuous constant of $\ell(w)$, $z_t = U^T w_t$ and $z^* = U^T w^*$.

The proof is also in Appendix 7.1. It is proved by showing that both the smooth part and the non-differentiable part satisfy the modified Lipchitz continuity.

## 4 Application to Conditional Random Fields with $\ell_1$ Penalty

In CRF problem, we are interested in learning a conditional distribution of labels $y \in \mathcal{Y}$ given observation $x \in \mathcal{X}$, where $\mathcal{Y}$ has application-dependent structure such as sequence, tree, or table in which label assignments have inter-dependency. The distribution is of the form

$$
P_w(y|x) = \frac{1}{Z_w(x)} \exp \left( \sum_{k=1}^d w_k f_k(y, x) \right),
$$

where $f_k$ is the feature functions, $w_k$ is the associated weight and $d$ is the number of feature functions. $Z_w(x)$ is the partition function. Given a training data set $\{(x_i, y_i)\}_{i=1}^N$, our goal is to find the optimal weights $w$ such that the following $\ell_1$-regularized negative log-likelihood is minimized.

$$
\min_w f(w) = \lambda \|w\|_1 - \sum_{i=1}^N \log P_w(y^{(i)}|x^{(i)})
$$

The gradient of $\ell(w)$ is given by

$$
\frac{\partial \ell(w)}{\partial w_k} = \sum_{i=1}^N \left( \sum_{y \in \mathcal{Y}} P_w(y|x^{(i)}) f_k(y, x^{(i)}) - f_k(y^{(i)}, x^{(i)}) \right)
$$

Since $|\mathcal{Y}|$, the number of possible values $y$ takes, can be exponentially large, the evaluation of $\ell(w)$ and gradient needs application-dependent oracles to conduct the summation over $\mathcal{Y}$. For example, in sequence labeling problem, a dynamic programming oracle, forward-backward algorithm, is usually employed to compute $\ell(w)$. Such an oracle can be very expensive. In Prox-QN algorithm for sequence labeling problem, the forward-backward algorithm takes $O(|\mathcal{Y}|^2 NT \times \exp)$ time, where $\exp$ is the time for the expensive exponential computation, $T$ is the sequence length and $\mathcal{Y}$ is the possible label set for a symbol in the sequence. Then given the obtained oracle, the evaluation of the partial gradients over the working set $\mathcal{A}$ has time complexity, $O(D_{nnz} |\mathcal{A}|T)$, where $D_{nnz}$ is the average number of instances related to a feature. Thus when $O(|\mathcal{Y}|^2 NT \times \exp + D_{nnz} |\mathcal{A}|T) > O(m^3 + m^2 |\mathcal{A}|)$, the gradients evaluation time will dominate.

The following theorem gives that the $\ell_1$-regularized CRF MLEs satisfy the CNSC-$\mathcal{T}$ condition.
Theorem 3. With $\ell_1$ penalty, the CRF loss function, $\ell(w) = -\sum_{i=1}^{N} \log P_w(y_i|x_i)$, satisfies the CNSC-\(T\) condition with $T = N^l$, where $N = \{v \in \mathbb{R}^d | \Phi^T v = 0\}$ is a constant subspace and $\Phi \in \mathbb{R}^{d \times (N|Y|)}$ is defined as below:

$$\Phi_{kn} = f_k(y_i, x^{(i)}) - E \left[ f_k(y, x^{(i)}) \right]$$

where $n = (i-1)|Y| + l$, $l = 1, 2, \ldots, |Y|$ and $E$ is the expectation over the conditional probability $P_w(y|x^{(i)})$.

The proof is given in Appendix 7.3.

According to the definition of CNSC-\(T\) condition, the $\ell_1$-regularized CRF MLEs don’t satisfy the classical strong-convexity condition when $N$ has nonzero members, which happens in the following two cases: (i) the exponential representation is not minimal [27], i.e. for any instance $i$ there exist a nonzero vector $a$ and a constant $b_i$ such that $\langle a, \phi(y_i, x^{(i)}) \rangle = b_i$; (ii) $d > N|Y|$. The first case holds in many problems, like the sequence labeling and hierarchical classification discussed in section 5 and the second case will hold in high-dimensional problems with a small label set $\mathcal{Y}$.

5 Related Methods

There have been several methods proposed for solving $\ell_1$-regularized $M$-estimators of the form in [8]. In this section, we will discuss these in relation to our method.

Orthant-Wise Limited-memory Quasi-Newton The popular (OWL-QN) introduced by Andrew and Gao [23] extends LBFGS to $\ell_1$-regularized problems. In each iteration, OWL-QN computes a generalized gradient called pseudo-gradient to determine the orthant and the search direction, then does a line search and a projection of the new iterate back to the orthant. Due to its fast convergence, it is widely implemented by many software packages, such as CRF++, CRFSuite and Wapiti, among others. But OWL-QN does not take advantage of the model sparsity in the optimization procedure, and moreover Yu et al. [22] have raised issues with its convergence proof.

Stochastic Gradient Descent (SGD) uses the gradient of a single sample as the search direction at each iteration. Thus, the computation for each iteration is very fast, which leads to fast convergence at the beginning. However, the convergence becomes slower than the second-order method when the iterate is close to the optimal solution. Recently, an $\ell_1$-regularized SGD algorithm proposed by Tsuruoka et al. [21] is claimed to have faster convergence than OWL-QN. It incorporates $\ell_1$-regularization by using a cumulative $\ell_1$ penalty, which is close to the $\ell_1$ penalty received by the parameter if it had been updated by the true gradient. Tsuruoka et al. do consider data sparsity, i.e. for each instance, only the parameters related to the current instance are updated. But they too do not take the model sparsity into account.

Coordinate Descent (CD) and Blockwise Coordinate Descent (BCD) are popular methods for $\ell_1$-regularized problem. In each coordinate descent iteration, it solves an one-dimension quadratic approximation of the objective function, which has a closed-form solution. It requires the second derivative with respect to the coordinate. But as discussed by Sokolovska et al., the exact second derivative in CRF problem is intractable. So they instead use an approximation of the second derivative, which can be computed efficiently by the same inference oracle queried for the gradient evaluation. However, pure CD is very expensive because it requires to call the inference oracle for the instances related to the current coordinate in each coordinate update. BCD alleviates this problem by grouping the parameters with the same $x$ feature into a block. Then each block update only needs to call the inference oracle once for the instances related to the current $x$. However, it cannot alleviate the large number of inference oracle calls unless the data is very sparse such that every instance appears only in a very few blocks.

Proximal Newton method has proven successful on problems of $\ell_1$-regularized logistic regression [13] and Sparse Invariance Covariance Estimation [5], where the Hessian-vector product can be cheaply re-evaluated for each update of coordinate. However, the Hessian-vector product for CI function like CRF requires query of inference oracle no matter how many coordinates are updated at a time [17], which then makes the coordinate update on quadratic approximation as expensive as coordinate update in the original problem. Our proximal quasi-Newton method avoids such problem by replacing Hessian with a low-rank matrix from BFGS update.

6 Numerical Experiments

We compare our approach, Prox-QN, with four other methods, Proximal Gradient (Prox-GD), OWL-QN [23], SGD [21] and BCD [16]. For OWL-QN, we directly use the OWL-QN optimizer developed by Andrew et al.\(^1\)

\(^1\)http://research.microsoft.com/en-us/downloads/b1eb1016-1738-4bd5-83a9-370c9d498a03/
and the memory size is set as $m = 10$, which is the same as in Prox-QN. For SGD, we implement the algorithm proposed by Tsuruoka et al. [21], and use cumulative $\ell_1$ penalty with learning rate $\eta_k = \eta_0/(1 + k/N)$, where $k$ is the SGD iteration and $N$ is the number of samples. For BCD, we follow Sokolovska et al. [16] but with three modifications. First, we add a line search procedure in each block update since we found it is required for convergence. Secondly, we apply shrinking strategy as discussed in Section 2.3, which makes the algorithm much faster. Thirdly, when the second derivative for some coordinate is less than $10^{-10}$, we set it to be $10^{-10}$ because otherwise the lack of $\ell_2$-regularization in our problem setting will lead to a very large new iterate. We evaluate the performance of the different methods on two problems, sequence labeling and hierarchical classification. The specific problems are discussed in the following subsections.

6.1 Sequence Labelling

In sequence labeling problem, $(x, y) = \{(x_t, y_t)\}_{t=1,\ldots,T}$ are $T$ pairs of sequence observations and the corresponding labels. Here we consider the optical character recognition (OCR) problem, which aims to recognize the handwriting words. The dataset was preprocessed by Taskar et al. [19] and was originally collected by Kassel [20], and contains 6877 words. The labels are 26 English letters and the observations are characters which are represented by images of 16 by 8 binary pixels as shown in Figure 1(a). We use degree 2 pixels as the raw features, which means all pixel pairs are considered. Therefore, the number of raw features is $d = 128 \times 127/2 + 128 + 1$, including a bias. For degree 2 features, $x_{tj} = 1$ only when both pixels are 1 and otherwise $x_{tj} = 0$. Here $x_{tj}$ is the $j$-th raw feature. For the feature functions, we use unigram feature functions $1(y_t = y, x_{tj} = 1)$ and bigram feature functions $1(y_t = y, y_{t+1} = y')$ with their associated weights, $\Theta_{y,y'} \in \mathbb{R}^{Y \times J}$ and $\Lambda_{y,y'} \in \mathbb{R}^{[Y \times Y]}$, respectively. So $w = \{\Theta_{y,y'}, \Lambda_{y,y'}\}$ and the total number of parameters, $d = |Y|^2 + |Y| \times J = 215,358$, where $|Y| = 26$. Using the above feature functions, the potential function can be specified as,

$$
\tilde{P}_w(y, x) = \exp \left\{ \langle \Lambda, \sum_{t=1}^{T} (e_{y_t} x_t^T) \rangle + \langle \Theta, \sum_{t=1}^{T-1} (e_{y_t} e_{y_{t+1}}^T) \rangle \right\}
$$

(10)

where $\langle \cdot, \cdot \rangle$ is the sum of element-wise product and $e_y \in \mathbb{R}^{|Y|}$ is an unit vector with 1 at y-th entry and 0 at other entries. The gradient and the inference oracle are given in the appendix.

In our experiment, $\lambda$ is set as 500, which leads to an optimal solution with 276 non-zero parameters. The learning rate $\eta_0$ for SGD is tuned to be $2 \times 10^{-4}$. In BCD, the unigram parameters are grouped into $J$ blocks according to the $x$ features while the bigram parameters are grouped into one block. The experiment is executed on 2.9GHz Intel Core i7 with 8G RAM and Mac OS. Our proximal quasi-Newton can be seen to be overwhelmingly faster than the other methods.

![Graphical model of OCR](image1)

![Relative Objective Difference](image2)

![Non-zero Parameters](image3)

**Figure 1: Sequence Labeling Problem**

6.2 Hierarchical Classification

In hierarchical classification problem, we have a label taxonomy, where the classes are grouped into a tree as shown in Figure 2(a). Here $y \in \mathcal{Y}$ is one of the leaf nodes and $x$ is the feature vector. If we have totally $K$ classes (number of nodes) and $J$ raw features, then the number of parameters is $d = K \times J$. Let $W \in \mathbb{R}^{K \times J}$ denote the

[2]http://www.seas.upenn.edu/~taskar/ocr/
weights. The feature function corresponding to \( W_{k,j} \) is 
\[
f_{k,j}(y, x) = 1[k \in \text{Path}(y)]x_j,
\]
where \( k \in \text{Path}(y) \) means class \( k \) is an ancestor of \( y \) or \( y \) itself. The potential function is 
\[
\tilde{P}_W(y, x) = \exp\left\{\sum_{k \in \text{Path}(y)} w_k^T x\right\}
\]
where \( w_k^T \) is the weights of \( k \)-th class, i.e. the \( k \)-th row of \( W \). The gradient and the inference oracle are given in the appendix.

The dataset is the training set from Task1 of LSHTC. It has 4,463 samples, each with \( J = 51,033 \) raw features. The hierarchical tree has 2,388 classes which includes 1,139 leaf labels. Thus, the number of the parameters \( d = 121,866,804 \). The feature values are scaled by svm-scale program in the LIBSVM package. We set \( \lambda = 2 \) and \( \eta_0 = 0.1 \). This \( \lambda \) leads to a solution with 2738 non-zeros. In BCD, parameters are grouped into \( J \) blocks according to the raw features. The experiment is executed on 2.93GHz Intel Xeon(R) X5570 with 100G RAM and Linux OS.

![Hierarchical Classification Problem](image)

**Figure 2: Hierarchical Classification Problem**

We plot the relative error \( (f(w_t) - f(w^*)) / f(w^*) \) and the number of non-zero parameters (on a log scale) against time in seconds. The results are dumped for every iteration. But for SGD, as the function evaluation takes extra time, we dump it every five \( N \) iterations. As both Figure 1(b),1(c) and Figure 2(b),2(c) show, Prox-QN achieves much faster convergence and moreover obtains a sparse model in much less time as well.

**References**

[1] Anonymous, Constant Nullspace Strong Convexity and Fast Convergence of Proximal Methods under High-Dimensional Settings, Submitted, 2014.

[2] X. Tang, K. Scheinberg, Efficiently Using Second Order Information in Large l1 Regularization Problems, arXiv:1303.6935, 2013.

[3] J. D. Lee, Y. Sun, and M. A. Saunders. Proximal newton-type methods for minimizing composite functions. In NIPS 2012.

[4] M. Schmidt, E. Van Den Berg, M.P. Friedlander, and K. Murphy. Optimizing costly functions with simple constraints: A limited-memory projected Quasi-Newton algorithm. In Int. Conf. Artif. Intell. Stat., 2009.

[5] C.-J. Hsieh, M. A. Sustik, I. S. Dhillon, and P. Ravikumar. Sparse inverse covariance estimation using quadratic approximation. In NIPS 2011.

[6] S. Boyd and L. Vandenberghe, Convex Optimization, Cambridge Univ. Press, Cambridge, U.K., 2003.

[7] P.-W. Wang and C.-J. Lin. Iteration Complexity of Feasible Descent Methods for Convex Optimization. Technical report, Department of Computer Science, National Taiwan University, Taipei, Taiwan, 2013.

[8] G.-X. Yuan, K.-W. Chang, C.-J. Hsieh, and C.-J. Lin. A comparison of optimization methods and software for large-scale 11-regularized linear classification. Journal of Machine Learning Research, 11:3183-3234, 2010.

[^1]: http://lshtc.iit.demokritos.gr/node/1
[9] A. Agarwal, S. Negahban, and M. Wainwright. Fast Global Convergence Rates of Gradient Methods for High-Dimensional Statistical Recovery. In NIPS 2010.

[10] K. Hou, Z. Zhou, A. M.-S. So, and Z.-Q. Luo. On the linear convergence of the proximal gradient method for trace norm regularization. In NIPS 2014.

[11] L. Xiao and T. Zhang. A proximal-gradient homotopy method for the l1-regularized least-squares problem. In ICML 2012.

[12] P. Tseng and S. Yun, A coordinate gradient descent method for nonsmooth separable minimization, Math. Prog. B. 117, 2009.

[13] G.-X. Yuan, C.-H. Ho, and C.-J. Lin, An improved GLMNET for l1-regularized logistic regression, Journal of Machine Learning Research, vol. 13, pp. 1999-2030, 2012.

[14] R.-E. Fan, K.-W. Chang, C.-J. Hsieh, X.-R. Wang, and C.-J. Lin, LIBLINEAR: A library for large linear classification, Journal of Machine Learning Research, vol. 9, pp. 1871-1874, 2008.

[15] A. J Hoffman. On approximate solutions of systems of linear inequalities. Journal of Research of the National Bureau of Standards, 1952.

[16] N. Sokolovska, T. Lavergne, Olivier Cappe and Francois Yvon. Efficient Learning of Sparse Conditional Random Fields for Supervised Sequence Labelling. arXiv:0909.1308 2009.

[17] Y. Tsuboi, Y. Unno, H. Kashima, N. Okazaki. Fast Newton-CG Method for Batch Learning of Conditional Random Fields, Proceedings of the Twenty-Fifth AAAI Conference on Artificial Intelligence, 2011.

[18] J. Nocedal and S. J. Wright. Numerical Optimization. Springer Series in Operations Research. Springer, New York, NY, USA, 2nd edition, 2006.

[19] B. Taskar, C. Guestrin, and D. Koller. Max-margin markov networks. In NIPS, 2003.

[20] R. Kassel. A Comparison of Approaches to On-line Handwritten Character Recognition. PhD thesis, MIT Spoken Language Systems Group, 1995.

[21] Y. Tsuruoka, J. Tsujii, and S. Ananiadou. Stochastic gradient descent training for l1- regularized log-linear models with cumulative penalty. In Proceedings of the Joint Conference of the 47th Annual Meeting of the ACL and the 4th International Joint Conference on Natural Language Processing of the AFNLP, pages 477-485, Suntec, Singapore, 2009.

[22] J. Yu, S.V.N. Vishwanathan, S. Gunter, and N. N. Schraudolph. A Quasi-Newton approach to nonsmooth convex optimization problems in machine learning. Journal of Machine Learning Research, 11:1-57, 2010.

[23] G. Andrew and J. Gao. Scalable training of ℓ1-regularized log-linear models. In ICML 2007.

[24] J.E. Dennis and J.J. More. A characterization of superlinear convergence and its application to Quasi-Newton methods. Math. Comp., 28(126):549-560, 1974.

[25] K. Scheinberg, X. Tang. Practical Inexact Proximal Quasi-Newton Method with Global Complexity Analysis. COR@L Technical Report at Lehigh University, arXiv:1311.6547 2013

[26] J. D. Lee, Y. Sun, and M. A. Saunders. Proximal Newton-type methods for minimizing composite functions. arXiv:1206.1623 2012

[27] M. J. Wainwright and M. I. Jordan. Graphical models, exponential families, and variational inference. Technical Report 649, Dept. Statistics, Univ. California, Berkeley, 2003
7 Appendix

7.1 Convergence Proof

7.1.1 Representing the problem in a reduced and compact space

Properties of CNSC-$\mathcal{T}$ condition
For $\ell(w)$ satisfying CNSC-$\mathcal{T}$ condition, we have $\ell(w) = \ell(\text{proj}_\mathcal{T}(w))$. As both $g$ and $H$ are in the $\mathcal{T}$ space, we have $g(w) = U^T g(\text{proj}_\mathcal{T}(w)) = g(\text{proj}_\mathcal{T}(w))$ and $H(w) = U^T H(\text{proj}_\mathcal{T}(w)) U U^T = H(\text{proj}_\mathcal{T}(w))$.

Objective formulation in the reduced space
Define $\ell(z) = \ell(Uz)$. Then if $z = U^T w$, we have $\hat{\ell}(z) = \ell(w)$, $\hat{g}(z) = U^T g(w)$ and $\hat{H}(z) = U^T H(w) U$, where $\hat{g}(z)$ and $\hat{H}(z)$ are the gradient and Hessian of $\hat{\ell}(z)$ respectively. Now $\hat{H}$ is positive definite with minimal eigenvalue $m$. The objective (1) can be re-formulated in the reduced space by

$$\min_z \hat{f}(z) = h(z) + \hat{\ell}(z),$$

where

$$h(z) = \min_{U^T w = z} \lambda\|w\|_1$$

$h(z)$ is also a non-differentiable convex function because it is the $\ell_1$ norm restricted to a linear subspace.

The optimal solution $z^*$ of (11) has the following relationship with the optimal solution $w^*$ of (1) ,

$$w^* = \arg\min_{U^T w = z^*} \lambda\|w\|_1$$

and $z^* = U^T w^*$

Lipchitz continuity in the reduced space
Throughout the paper, we assume the Hessian of $\ell(w)$ has Lipchitz continuity with constant $L_H$. According to the Lipchitz continuity,

$$\|H(w_2)(w_1 - w_2) - (g(w_1) - g(w_2))\| \leq \frac{L_H}{2} \|w_1 - w_2\|^2$$

In the corresponding reduced space, the Lipchitz continuity also holds with the same constant .

$$\|\hat{H}(z_2)(z_1 - z_2) - (\hat{g}(z_1) - \hat{g}(z_2))\| \leq \frac{L_H}{2} \|z_1 - z_2\|^2$$

BFGS update formula in the reduced space
If $B_0$ is in the $\mathcal{T}$ space, $B_t$ is also in the $\mathcal{T}$ space. This can be shown by re-formulating the BFGS update and mathematical induction,

$$B_t = U \hat{B}_{t-1} U^T - \frac{U \hat{B}_{t-1} U^T s_{t-1} s_{t-1}^T U \hat{B}_{t-1} U^T}{s_{t-1}^T U \hat{B}_{t-1} U^T s_{t-1}} + \frac{U U^T \hat{y}_{t-1} \hat{y}_{t-1}^T U U^T}{\hat{y}_{t-1}^T U U^T s_{t-1}}$$

Thus

$$\hat{B}_t = \hat{B}_{t-1} - \frac{\hat{B}_{t-1} \hat{s}_{t-1} \hat{s}_{t-1}^T \hat{B}_{t-1}}{\hat{s}_{t-1}^T \hat{B}_{t-1} \hat{s}_{t-1}} + \frac{\hat{y}_{t-1} \hat{y}_{t-1}^T}{\hat{y}_{t-1} \hat{s}_{t-1}}$$

where $\hat{s} = U^T s$, $\hat{y} = U^T y$ and $U \hat{B}_t U^T = B_t$. It can be proved that $\hat{B}_t$ generated in (15) is positive definite provided $\hat{y}^T \hat{s} > 0$ [18]. In addition, we assume $m\|z\|^2 \leq z^T B_t z \leq M\|z\|^2$ for any $z \in \mathbb{R}^d$, i.e. $B_t$ satisfies the CNSC-$\mathcal{T}$ condition.

Iterate in the reduced space
The potential new iterate $w^+$ is

$$w^* = \arg\min_w \lambda\|w\|_1 + \frac{1}{2}(v - w_t)^T B_t(v - w_t) + g_t^T(v - w_t)$$

In the reduced space, the potential new iterate (16) can be represented by,

$$z^* = \arg\min_x h(x) + \frac{1}{2}(x - z_t)^T \hat{B}_t(x - z_t) + \hat{g}_t^T(x - z_t)$$
z^+ and w^+ also satisfy Equation (18), i.e.

$$w^+ = \arg\min_{U^T w = z^+} \|w\|_1$$

(18)

In this paper, we consider the convergence phase when \(z_t\) is close enough to the optimum such that the unit step size is always chosen, i.e. \(z_{t+1} = z^+\) \(\text{(26)}\).

### 7.1.2 Quadratic Convergence of Proximal Newton Algorithm and Dennis-More Criterion

**Lemma 1** (Quadratic Convergence of Prox-Newton). For \(\ell(z)\) satisfying Lipchitz-continuous second derivative \(\hat{H} = \nabla^2 \ell(z)\) with \(m\|z\|^2 \leq z^T \hat{H} z\) for any \(z \in \mathbb{R}^d\), the sequence \(\{z_t\}_{t=1}^\infty\) produced by proximal Newton Method (replacing \(\hat{B}_t\) by \(\hat{H}_t\) in \((17)\)) has

$$\|z_{t+1} - z^*\| \leq \frac{L_H}{2m}\|z_t - z^*\|^2,$$

where \(z^*\) be the optimal solution of \((11)\) and \(L_H\) is the Lipchitz constant for \(\hat{H}\).

**Proof.** The conditions in this lemma satisfies those required by Theorem 3.4 in \(\text{(26)}\), which we can directly follow.

**Lemma 2.** If \(B_0 = U\tilde{B}_0 U^T\) satisfies CNSC-T condition, then \(\tilde{B}_t\) generated by \((15)\) satisfies the Dennis-More criterion \(\text{(24)}\), namely,

$$\lim_{t \to \infty} \frac{\|\tilde{B}_t - \tilde{H}(z^*)\|}{\|z_{t+1} - z_t\|} = 0,$$

where \(U\tilde{H}(z^*)^T = \nabla^2 \ell(z^*)\) and \(z^*\) is the optimal solution of the new objective \((11)\).

**Proof.** The Lipchitz continuity of \(H(w)\) implies the Lipchitz continuity of \(\hat{H}(z)\):

$$\|\hat{H}(z_1) - \hat{H}(z_2)\| = \|U^T (H(w_1) - H(w_2))U\|
\leq \|H(w_1) - H(w_2)\|
= \|H(Uz_1) - H(Uz_2)\|
\leq L_H\|z_1 - z_2\|$$

where the last inequality is from the Lipchitz continuity of \(H(w)\).

It can also be verified that the BFGS update in \(T\) space \((15)\) guarantees the secant equation, i.e. \(\tilde{B}_t \delta_{t-1} = \tilde{y}_{t-1}\).

Now the theorem follows from Theorem 6.6 of \(\text{(18)}\) given the assumption, \(\sum_{t=0}^\infty \|z_t - z^*\| < \infty\).

### 7.1.3 Asymptotic Superlinear Convergence

**Proof of Theorem 1**

**Proof.** Assuming \(B_t\) satisfies CNSC-T condition, \(\tilde{B}_t\) satisfies \(m\|z\|^2 \leq z^T \tilde{B}_t z \leq M\|z\|^2\) for any \(z \in \mathbb{R}^d\). The Lipchitz-continuous \(\hat{H}\) implies Lipchitz-continuity of \(\hat{H}\). Therefore this theorem follows from Theorem 3.7 in \(\text{(26)}\), Lemma 2 and Lemma 1 by applying the algorithm in the reduced space.

**Proof of Theorem 2**

**Proof.** We prove this theorem by showing \(|\ell(w_t) - \ell(w^*)| \leq L_\ell\|z_t - z^*\|\) and \(\|w_t\|_1 - \|w^*\|_1 \leq \|z_t - z^*\|\).

The first part is given by,

$$|\ell(w_t) - \ell(w^*)| = |\ell(UU^T w_t) - \ell(UU^T w^*)| \leq L_\ell\|UU^T (w_t - w^*)\| = L_\ell\|z_t - z^*\|$$

where the inequality comes from the Lipchitz-continuity of \(\ell(w)\). Since each iterate satisfies \((18)\), we have \(\|w_t\|_1 \leq \|UU^T w_t + (I - UU^T) w^*\|_1\). Moreover, due to the Lipchitz-continuity of \(\ell_1\) norm, which is \(\|w\|_1 - \|v\|_1 \leq \sqrt{d}\|w - v\|\), we have,

$$\|UU^T w_t + (I - UU^T) w^*\|_1 \leq \|w^*\|_1 + \sqrt{d}\|UU^T w_t - UU^T w^*\|
\leq \|w^*\|_1 + \sqrt{d}\|z_t - z^*\|$$

\(\square\)
7.2 Algorithm Details

Algorithm 2 Proximal Quasi-Newton Algorithm

**Input:** Observations \( \{x^{(i)}\}_{i=1,2,...,N} \), labels \( \{y^{(i)}\}_{i=1,2,...,N} \), termination criterion \( \epsilon \), scalar \( \lambda \) and LBFGS memory size \( m \).

**Output:** \( w^* \) converging to \( \arg\min_w f(w) \)

1: Initialize \( \gamma = 1, w \leftarrow 0, g \leftarrow \partial f(w) / \partial w \), working set \( A \leftarrow \{1,2,...,d\} \), \( M \leftarrow \infty \), and \( S, Y, Q, \hat{Q} \leftarrow \phi \).

2: for \( n = 0, 1, \ldots \) do

3: \( \hat{A} \leftarrow A, A \leftarrow \phi, M \leftarrow 0 \) # Shrink the working set

4: for \( j \) in \( \hat{A} \) do

5: \( \partial_j f(w) = \begin{cases} g_j + \text{sgn}(w_j)\lambda & \text{if } w_j \neq 0 \\ \text{sgn}(g_j) \max\{|g_j| - \lambda, 0\} & \text{if } w_j = 0 \end{cases} \) \hspace{1cm} (19)

6: if \( w_j \neq 0 \) or \( |g_j| - \lambda + M/N > 0 \) then

7: \( \hat{A} \leftarrow A \cup j, M \leftarrow \max\{M, |\partial_j f|\} \)

8: end if

9: end for

10: \( \hat{M} \leftarrow M \)

11: if Shrinking stopping criterion attained then # Check stopping criterion

12: if Stopping criterion attained and \( |A| = d \) then

13: return \( w \)

14: else

15: \( g \leftarrow \partial f(w) / \partial w, A \leftarrow \{1,2,...,d\} \) and \( S, Y, Q, \hat{Q} \leftarrow \phi \)

16: Update shrinking stopping criterion and then continue

17: end if

18: end if

19: \( d \leftarrow 0, \hat{d} \leftarrow 0 \)

20: Compute \( inner_{iter} = \min\{\max\_inner, \lfloor \frac{d}{|A|} \rfloor \} \)

21: for \( p = 1, 2, \ldots inner_{iter} \) do # Solve inner problem

22: for \( j \) in \( A \) do

23: \( B_{jj} = \gamma - q_j^T q_j, (B \hat{d})_j = \gamma d_j - q_j^T d \)

24: Compute \( z \) according to Equation (4)

25: \( d_j \leftarrow d_j + z, \hat{d} \leftarrow \hat{d} + z \hat{q}_j \)

26: end for

27: end for

28: for \( \alpha = \beta^0, \beta^1, \ldots \) do # Conduct line search

29: if \( f(w + \alpha d) \leq f(w) + \alpha \sigma(\lambda \|w + \alpha d\| - \lambda \|w\| + g^T d) \) then

30: break

31: end if

32: end for

33: for \( j \) in \( A \) do

34: \( g_j^{\text{new}} = \partial f(w) / \partial w_j, y_j = g_j^{\text{new}} - g_j, s_j = \alpha d_j, g_j = g_j^{\text{new}} \)

35: end for

36: Update \( S, Y \) and \( \hat{Q} \) just on the rows corresponding to \( A \).

37: Update \( \gamma, D, L, S^T S \) where computing the inner product between \( s \) and another vector sum just over \( A \).

38: Update \( R \) and then update \( \hat{Q} \) just on the columns corresponding to \( A \).

39: end for
Theorem holds because of the following four reasons.

1) \[ H = \Phi D \Phi, \]

Here \( D \in \mathbb{R}^{(N|\mathcal{Y}|) \times (N|\mathcal{Y}|)} \) is a diagonal matrix with diagonal elements \( D_{nn} = P_w(y_i|x^{(i)}) \), where \( n = (i - 1)|\mathcal{Y}| + l \) and \( l = 1, 2, \ldots, |\mathcal{Y}| \). \( \Phi \) is a \( d \times (N|\mathcal{Y}|) \) matrix whose column \( n \) is defined as \( \Phi_n = \phi(y_i, x^{(i)}) - E[\phi(y_i, x^{(i)})] \) for \( n = (i - 1)|\mathcal{Y}| + l \).

The theorem holds because of the following four reasons.

a. \( \mathcal{N} \) is constant with respect to \( w \).

\( \mathcal{N} \) is equivalent to

\[ \mathcal{N} = \{ a \in \mathbb{R}^d | \forall i, \exists \text{ some constant } b_i, \langle a, \phi(y_i, x^{(i)}) \rangle = b_i \text{ for } \forall y \} \tag{21} \]

Thus \( \mathcal{N} \) is independent on \( w \) and so is \( \mathcal{T} \).

b. \( \ell(w) \) depends only on \( z = \text{proj}_T(w) \).

Let \( w = z + u \). So \( u \in \mathcal{N} \).

\[ P_w(y^{(i)}|x^{(i)}) = \frac{\exp \left\{ \langle u, \phi(y^{(i)}, x^{(i)}) \rangle \right\}}{\sum_y \exp \left\{ \langle u, \phi(y^{(i)}, x^{(i)}) \rangle \right\}} = \frac{\exp \left\{ \langle z, \phi(y^{(i)}, x^{(i)}) \rangle \right\} \exp \left\{ \langle u, \phi(y^{(i)}, x^{(i)}) \rangle \right\}}{\sum_y \exp \left\{ \langle z, \phi(y^{(i)}, x^{(i)}) \rangle \right\} \exp \left\{ \langle u, \phi(y^{(i)}, x^{(i)}) \rangle \right\}} = \frac{\exp \left\{ \langle z, \phi(y^{(i)}, x^{(i)}) \rangle \right\}}{\sum_y \exp \left\{ \langle z, \phi(y^{(i)}, x^{(i)}) \rangle \right\}} \]

The last equality comes from the character of \( \mathcal{N} \), Equation (21).

c. The first property \[5\] holds.

\( D_{nn} \to 0 \) iff \( \|w\|_1 \to \infty \) which is prohibited by \( \ell_1 \) penalty. Thus there exists \( m_p > 0 \) such that \( D_{nn} \geq m_p \) for any \( u \). Hence, the positive definiteness of \( H \) is determined by \( \Phi \).

We have for any \( v \in \mathcal{T} \),

\[ m_p \lambda_{mn}(\Phi \Phi^T)\|v\|^2 \leq m_p v^T \Phi \Phi^T v \leq v^T H v \leq v^T \Phi \Phi^T v \leq \lambda_{max}(\Phi \Phi^T)\|v\|^2 \]

where \( \lambda_{min}(\Phi \Phi^T) \) is the minimum nonzero eigenvalue of \( \Phi \Phi^T \) and \( \lambda_{max}(\Phi \Phi^T) \) is the maximum eigenvalue of \( \Phi \Phi^T \).

d. The second property \[5\] holds.

This property directly follows the definition of \( \mathcal{N} \).

\[ \square \]

7.4 Gradient evaluation in sequence labeling and hierarchical classification

7.4.1 Sequence labeling

The gradients of \( \ell(w) \) for sequence labeling problem are,

\[ \frac{\partial \ell(\Theta, \Lambda)}{\partial \Theta_{y,i}} = \sum_{i=1}^N \sum_{t=1}^{T^{(i)}} \left( P_w(y_t = y_i|x^{(i)}) - 1 \left[ y^{(i)}_t = y \right] \right) x^{(i)}_{ij} \tag{22} \]

\[ \frac{\partial \ell(\Theta, \Lambda)}{\partial \Lambda_{y,y'}} = \sum_{i=1}^N \sum_{t=1}^{T^{(i)}-1} \left( P_w(y_t = y, y_{t+1} = y'_i|x^{(i)}) - 1 \left[ y^{(i)}_t = y, y^{(i)}_{t+1} = y' \right] \right) \tag{23} \]
The forward-backward algorithm is a popular inference oracle for evaluating the marginal probability in Equation (22) and (23). In our OCR model, the forward-backward algorithm is

\[
\begin{align*}
\alpha_1(y) &= \exp(\Theta_y^T x_1) \\
\alpha_{t+1}(y) &= \sum_{y'} \alpha_t(y') \exp(\Theta_y^T x_{t+1} + \Lambda_{y',y}) \\
\beta_T(y) &= 1 \\
\beta_t(y') &= \sum_y \beta_{t+1}(y) \exp(\Theta_y^T x_{t+1} + \Lambda_{y',y})
\end{align*}
\]

where \(\Theta_y^T\) is the \(y\)-th row of the matrix \(\Theta\). Then the marginal conditional probabilities are given by

\[
P_w(y_t = y', y_{t+1} = y | x) = \frac{1}{Z_w(x)} \alpha_t(y') \exp(\Theta_y^T x_{t+1} + \Lambda_{y',y}) \beta_{t+1}(y),
\]

where the normalization factor \(Z_w(x)\) can be computed by \(\sum_y \alpha_t(y)\).

### 7.4.2 Hierarchical classification

The partial gradients of \(\ell(W)\) for hierarchical classification problem are,

\[
\frac{\partial \ell(W)}{\partial W_{k,j}} = \sum_{i=1}^{N} \left( \sum_{y\in Y} 1[k \in \text{Path}(y)] P_W(y|x^{(i)}) - 1[k \in \text{Path}(y^{(i)})] \right) x_j^{(i)}
\]

They can be evaluated by the downward-upward algorithm. Let \(\alpha(k)\) and \(\beta(k)\) be the downward message and upward message respectively.

\[
\begin{align*}
\alpha(\text{root}) &= w_{\text{root}}^T x \\
\alpha(k) &= \alpha(\text{parent}(k)) + w_k^T x \\
\beta(k) &= \alpha(k) / \sum_{y \in Y} \alpha(y) \quad \text{if } k \text{ is a leaf node} \\
\beta(k) &= \sum_{k' \in \text{children}(k)} \beta(k') \quad \text{if } k \text{ is a non-leaf node}
\end{align*}
\]

So we have

\[
\frac{\partial \ell(W)}{\partial W_{k,j}} = \sum_{i=1}^{N} \left( \beta^{(i)}(k) - 1[k \in \text{Path}(y^{(i)})] \right) x_j^{(i)}
\]

(24)