Split Bregman method for large scale fused Lasso

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Abstract: Ordering of regression or classification coefficients occurs in many real-world applications. Fused Lasso exploits this ordering by explicitly regularizing the differences between neighboring coefficients through an ℓ_1 norm regularizer. However, due to nonseparability and nonsmoothness of the regularization term, solving the fused Lasso problem is computationally demanding. Existing solvers can only deal with problems of small or medium size, or a special case of the fused Lasso problem in which the predictor matrix is identity matrix. In this paper, we propose an iterative algorithm based on split Bregman method to solve a class of large-scale fused Lasso problems, including a generalized fused Lasso support vector classifier. We derive our algorithm using augmented Lagrangian method and prove its convergence properties. The performance of our method is tested on both artificial data and real-world applications including proteomic data from mass spectrometry and genomic data from array CGH. We demonstrate that our method is many times faster than the existing solvers, and show that it is especially efficient for large p, small n problems.

Keywords and phrases: Fused Lasso, Bregman iteration, ℓ_1 -norm, Mass spectrometry, Array CGH.

1. Introduction

Regularization terms that encourage sparsity in coefficients are increasingly being used in regression and classification procedures. One widely used example is the Lasso procedure for linear regression, which minimizes the usual sum of squared errors, but additionally penalizes the ℓ_1 norm of the regression coefficients. Because of the non-differentiability of the ℓ_1 norm, the Lasso procedure tends to shrink the regression coefficients toward zero and achieves sparseness. Fast and efficient algorithms are available to solve Lasso with as many as millions of variables, which makes it an attractive choice for many large-scale real-world applications.

The fused Lasso method introduced by Tibshirani et al. [1] is an extension of Lasso, and considers the situation where there is certain natural ordering in regression coefficients. Fused Lasso takes this natural ordering into account by placing an additional regularization term on the differences of "neighboring" coefficients. Consider the linear regression of $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, where $\mathbf{x}_i = (x_{i1}, \ldots, x_{ip})^T$ are the predictor variables and y_i are the responses. (We assume x_{ij}, y_i are standardized with zero mean and unit variance across different observations.) Fused Lasso finds the coefficients of linear regression by minimizing the following loss function

$$\Phi(\beta) = \frac{1}{2} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda_1 \sum_{i=1}^{p} |\beta_i| + \lambda_2 \sum_{i=2}^{p} |\beta_i - \beta_{i-1}|,$$
(1)

where the regularization term with parameter λ_1 encourages the sparsity of the regression coefficients, while the regularization term with parameter λ_2 shrinks the differences between neighboring coefficients toward zero. As such, the method achieves both sparseness and smoothness in the regression coefficients.

Regression or classification variables with some inherent ordering occur naturally in many real-world applications. In genomics, chromosomal features such as copy number variations (CNV), epigenetic modification patterns, and genes are ordered naturally by their chromosomal locations. In proteomics, molecular fragments from mass spectrometry (MS) measurements are ordered by their mass-to-charge ratios (m/z). In dynamic gene network inference, gene regulatory networks from developmentally closer cell types are more similar than those from more distant cell types [2]. Fused Lasso exploits these natural ordering, so, not surprisingly, it has found applications in these areas particularly suitable. For example, Tibshirani and Wang successfully applied fused Lasso to detect DNA copy number variations in tumor samples using array comparative genomic hybridization (CGH) data [3]. Tibshirani et al. used fused Lasso to select proteomic features that can separate tumor vs normal samples [1]. In addition to the application areas mentioned above, fused Lasso or the extension of it has also found applications in a number of other areas, including image denoising, social networks [2], quantitative trait network analysis [4], etc.

The loss function in (1) is strictly convex, so a global optimal solution is guaranteed to exist. However, finding the optimal solution is computationally challenging due to the nondifferentiability of $\Phi(\beta)$. Existing methods circumvent the nondifferentiability of $\Phi(\beta)$ by introducing 2p-1 additional variables and converting the unconstrained optimization problem into a constrained one with 6p-1 linear inequality constraints. Standard convex optimization tools such as SQOPT [5] and CVX [6] can then be applied. Because of the large number of variables introduced, these methods are computationally demanding in terms of both time and space, and, in practice, have only been able to solve fused Lasso problems with small or medium sizes.

Component-wise coordinate descent has been proposed as an efficient approach for solving many l_1 regularized convex optimization problems, including Lasso, grouped Lasso, elastic nets, graphical Lasso, logistic regression, etc [7]. However, coordinate descent cannot be applied to the fused Lasso problem because the variables in the loss function $\Phi(\beta)$ are nonseparable due to the second regularization term, and as such, convergence is not guaranteed [8].

For a special class of fused Lasso problems, named fused Lasso signal approximator (FLSA), where the predictor variables $x_{ij} = 1$ for all i = j and 0 otherwise, there are algorithms available to solve it efficiently. A key observation of FLSA first noticed by Friedman et al. is that for fixed λ_1 , increasing λ_2 can only cause pairs of variables to fuse and they become unfused for any larger values of λ_2 . This observation allows Friedman et al. to develop a fusion algorithm to solve FLSA for a path of λ_2 values by keeping track of fused variables and using coordinate descent for component-wise optimization. The fusion algorithm was later extended and generalized by Hoefling [9]. However, for the fusion algorithm to work, the solution path as a function of λ_2 has to be piecewise linear , which is not true for the general fused Lasso problem [10]. As such, these algorithms are not applicable to the general fused Lasso case.

In this paper, we propose a new method based on the split Bregman iteration for solving the general fused Lasso problem. Although the Bregman iteration was an old technique proposed in the sixties [11, 12], it gained significant interest only recently after Osher and his coauthors demonstrated its high efficiency for image restoration [13, 14, 15]. Most recently, it has also been shown to be an efficient tool for compressed sensing [16, 17, 18], matrix completion [19] and low rank matrix recovery [20]. In the following, we will show that the general fused Lasso problem can be reformulated so that split Bregman iteration can be readily applied.

The rest of the paper is organized as follows. In Section 2, we derive algorithms for a class of fused Lasso problems from augmented Lagrangian function including SBFLasso for general fused Lasso, SBFLSA for FLSA and SBFLSVM for fused Lasso support vector classifier. The convergence properties of our algorithms are also presented. We demonstrate the performance and effectiveness of the algorithm through numerical examples in Section 3, and describe additional implementation details. Algorithms described in this paper are implemented in Matlab and are freely available from the authors.

2. Algorithms

2.1. Split Bregman iteration for a generalized fused Lasso problem

We first describe our algorithm in a more general setting than the one described in (1). Instead of the quadratic error function, we allow the error function to be any convex function of the regression coefficients. In addition, we relax the assumption that the coefficients should be ordered along a line as in (1), and allow the ordering to be specified arbitrarily, e.g., according to a graph. For the generalized fused Lasso, we find β by solving the following unconstrained optimization problem

$$\min_{\beta} V(\beta) + \lambda_1 \|\beta\|_1 + \lambda_2 \|L\beta\|_1, \tag{2}$$

where $V(\beta) = V(\beta; X, y)$ is the error term, the regularization term with parameter λ_1 encourages the sparsity of β as before, and the regularization term with parameter λ_2 shrinks the differences between neighboring variables as specified in matrix L toward zero. We assume L is an $m \times p$ matrix. In the standard fused Lasso in (1), L is simply a $(p-1) \times p$ matrix with zeros entries everywhere except 1 in the diagonal and -1 in the superdiagonal. The unconstrained problem (2) can be reformulated into an equivalent constrained problem

$$\min_{\beta} \quad V(\beta) + \lambda_1 \|a\|_1 + \lambda_2 \|b\|_1$$
s.t. $a = \beta$
 $b = L\beta$. (3)

Although split Bregman methods originated from Bregman iterations [16, 13, 18, 21, 14, 15], it is more convenient to derive the split Bregman method for the generalized Lasso using the augmented Lagrangian method [22, 23].

Note that the Lagrangian function of (3) is

$$\hat{\mathcal{L}}(\beta, a, b, u, v) = V(\beta) + \lambda_1 ||a||_1 + \lambda_2 ||b||_1 + \langle u, \beta - a \rangle + \langle v, L\beta - b \rangle,$$
(4)

where $u \in \mathbb{R}^p$ is a dual variable corresponding to the linear constraint $\beta = a, v \in \mathbb{R}^m$ is a dual variable corresponding to the linear constraint $L\beta = b, \langle \cdot, \cdot \rangle$ denotes the standard inner product in Euclidean space. The augmented Lagrangian function of (3) is similar to the (4) except for adding two terms $\frac{\mu_1}{2} \|\beta - a\|_2^2 + \frac{\mu_2}{2} \|L\beta - b\|_2^2$ to penalize the violation of linear constraints $\beta = a$ and $L\beta = b$. That is,

$$\mathcal{L}(\beta, a, b, u, v) = V(\beta) + \lambda_1 \|a\|_1 + \lambda_2 \|b\|_1 + \langle u, \beta - a \rangle + \langle v, L\beta - b \rangle + \frac{\mu_1}{2} \|\beta - a\|_2^2 + \frac{\mu_2}{2} \|L\beta - b\|_2^2,$$
(5)

where $\mu_1 > 0$ and $\mu_2 > 0$ are two parameters.

Consider the problem of finding a saddle point $(\beta^*, a^*, b^*, u^*, v^*)$ of the augmented Lagrangian function $\mathcal{L}(\beta, a, b, u, v)$ such that

$$\mathcal{L}(\beta^*, a^*, b^*, u, v) \le \mathcal{L}(\beta^*, a^*, b^*, u^*, v^*) \le \mathcal{L}(\beta, a, b, u^*, v^*)$$
(6)

for all β , a, b, u and v. It can be shown that β^* is an optimal solution of (2) if and only if $(\beta^*, a^*, b^*, u^*, v^*)$ solves the above saddle point problem for some a^* , b^* , u^* , and v^* .

We solve the saddle point problem through an iterative algorithm by alternating between the primal and the dual optimization as follows

$$\begin{cases} \text{Primal}: & (\beta^{k+1}, a^{k+1}, b^{k+1}) = \arg\min_{\beta, a, b} \mathcal{L}(\beta, a, b, u^k, v^k) \\ \text{Dual}: & u^{k+1} = u^k + \delta_1(\beta^{k+1} - a^{k+1}), \ v^{k+1} = v^k + \delta_2(L\beta^{k+1} - b^{k+1}) \end{cases}$$
(7)

where the first step updates the primal variables based on the current estimate of u^k and v^k , while the second step updates the dual variables based on the current estimate of the primal variables. Since the augmented Lagrangian function is linear in u and v, updating the dual variables are relatively easy and we use gradient ascent algorithm with step size δ_1 and δ_2 .

The efficiency of the iterative algorithm (7) lies on whether the primal problem can be solved quickly. The augmented Lagrangian function \mathcal{L} still contains nondifferentiable terms. But different from the original objective function in (2), the ℓ_1 induced nondifferentiability has now been transferred from terms involving β to terms involving a and b only. Moreover, the nondifferentiable terms involving a and b are now completely decoupled, and thus we can solve the primal problem by alternating minimization of β , a and b,

$$\begin{cases} \beta^{k+1} = \arg\min_{\beta} V(\beta) + \langle u^{k}, \beta - a^{k} \rangle + \langle v^{k}, L\beta - b^{k} \rangle + \frac{\mu_{1}}{2} \|\beta - a^{k}\|_{2}^{2} + \frac{\mu_{2}}{2} \|L\beta - b^{k}\|_{2}^{2} \\ a^{k+1} = \arg\min_{a} \lambda_{1} \|a\|_{1} + \langle u^{k}, \beta^{k+1} - a \rangle + \frac{\mu_{1}}{2} \|\beta^{k+1} - a\|_{2}^{2} \\ b^{k+1} = \arg\min_{b} \lambda_{2} \|b\|_{1} + \langle v^{k}, L\beta^{k+1} - b \rangle + \frac{\mu_{2}}{2} \|L\beta^{k+1} - b\|_{2}^{2}. \end{cases}$$
(8)

Minimization of a and b in (8) can be done efficiently using soft thresholding, because the objective functions are quadratic and nondifferentiable terms are completely separable. Let \mathcal{T}_{λ} be a soft thresholding operator defined on vector space and satisfying

$$\mathcal{T}_{\lambda}(w) = [t_{\lambda}(w_1), t_{\lambda}(w_2), \dots, \dots]^T, \quad \text{with } t_{\lambda}(w_i) = \operatorname{sgn}(w_i) \max\{0, |w_i| - \lambda\}.$$
(9)

Using the soft thresholding operator, the optimal solution of a and b in (8) can be written as

$$a^{k+1} = \mathcal{T}_{\mu_1^{-1}\lambda_1}(\beta^{k+1} + \mu_1^{-1}u^k) \quad \text{and} \quad b^{k+1} = \mathcal{T}_{\mu_2^{-1}\lambda_2}(L\beta^{k+1} + \mu_2^{-1}v^k).$$
(10)

Therefore, the efficiency of the iterative algorithm depends entirely on whether the minimization of β in (8) can be done efficiently. If $V(\beta)$ is a quadratic function as in the standard fused Lasso, the optimal solution β^{k+1} can be found analytically.

In theory, the alternate minimization between the primal variables needs to run multiple times until convergence. However, we do not have to completely solve the primal problem since it is only one step of the overall iterative algorithm. Our algorithm uses only one alternation. Overall, we propose Algorithm 1 for solving the saddle point problem (6), and consequently the problem (2).

Algorithm 1: Split Bregman method for the generalized Fused Lasso (2)

 $\begin{array}{l} \mbox{Initialize } \beta^0, \, a^0, b^0, u^0, \, \mbox{and } v^0. \\ \mbox{repeat} \\ 1) \ \beta^{k+1} = \arg\min_\beta V(\beta) + \langle u^k, \beta - a^k \rangle + \langle v^k, L\beta - b^k \rangle + \frac{\mu_1}{2} \|\beta - a^k\|_2^2 + \frac{\mu_2}{2} \|L\beta - b^k\|_2^2 \\ 2) \ a^{k+1} = \mathcal{T}_{\mu_1^{-1}\lambda_1}(\beta^{k+1} + \mu_1^{-1}u^k) \\ 3) \ b^{k+1} = \mathcal{T}_{\mu_2^{-1}\lambda_2}(L\beta^{k+1} + \mu_2^{-1}v^k) \\ 4) \ u^{k+1} = u^k + \delta_1(\beta^{k+1} - a^{k+1}) \\ 5) \ v^{k+1} = v^k + \delta_2(L\beta^{k+1} - b^{k+1}) \\ \mbox{until} \\ \mbox{Convergence} \end{array}$

The convergence property of Algorithm 1 is shown in the following theorem, which we prove in the Supplementary Info.

Theorem 1. Suppose there exists at least one solution β^* of (2). Assume $V(\beta)$ is convex, $0 < \delta \leq \mu_1$, $0 < \delta_2 \leq \mu_2$, and $\lambda_1 > 0$, $\lambda_2 > 0$. Then the following property for the split Bregman iteration in Algorithm 1 holds:

$$\lim_{k \to \infty} V(\beta) + \lambda_1 \|\beta^k\|_1 + \lambda_2 \|L\beta^k\|_1 = V(\beta^*) + \lambda_1 \|\beta^*\|_1 + \lambda_2 \|L\beta^*\|_1.$$
(11)

Furthermore,

$$\lim_{k \to \infty} \|\beta^k - \beta^*\| = 0 \tag{12}$$

whenever (2) has a unique solution.

Note that the condition for the convergence in Theorem 1 is quite easy to satisfy. λ_1, λ_2 are regularization parameters and should always be larger than zero. So as long as $0 < \delta_1 \leq \mu_1$ and $0 < \delta_2 \leq \mu_2$, the algorithm converges. In our implementation, we just choose $\delta_1 = \mu_1$ and $\delta_2 = \mu_2$.

2.2. Split Bregman for the standard fused Lasso (SBFLasso)

Next we apply Algorithm 1 to solve the standard fused Lasso problem (1), which constitutes a special case of the generalized fused Lasso problem with

$$V(\beta; X, y) = \frac{1}{2} ||X\beta - y||_2^2$$

and

$$L\beta = (\beta_2 - \beta_1, \beta_3 - \beta_2, \dots, \beta_p - \beta_{p-1})^T,$$
(13)

where $X = (x_{i,j})_{i=1,j=1}^{n,p}$ and $y = (y_1, \dots, y_n)^T$.

The objective function on minimizing β in Algorithm 1 is now quadratic and differentiable, and thus the optimal solution can be found by solving a set of linear equations:

$$(X^T X + \mu_1 I + \mu_2 L^T L)\beta^{k+1} = X^T y + \mu_1 (a^k - \mu_1^{-1} u^k) + \mu_2 L^T (b^k - \mu_2^{-1} v^k),$$
(14)

while the other four steps in Algorithm 1 are easy to implement and can be computed quickly. So the efficiency of the algorithm largely depends on how fast the linear equations can be solved. Matrix $D = X^T X + \mu_1 I + \mu_2 L^T L$ is a $p \times p$ matrix, independent of the optimization variables. For small p, we can invert D and store D^{-1} in the memory, so the linear equations can be solved with minimal cost. However, for large p, we will need to numerically solve the linear equations at each iteration.

The matrix $P = \mu_1 I + \mu_2 L^T L$ occurring in (14) is a tridiagonal positive definite matrix, and as such, the linear equation $(\mu_1 I + \mu_2 L^T L)\mathbf{x} = \mathbf{g}$ can be solved efficiently for any $\mathbf{x}, \mathbf{g} \in \mathbb{R}^p$, requiring only order of p operations. More specifically, there exists a matrix \hat{L} satisfying $\hat{L}_{ij} = 0$ for all $i \neq j$ and $i \neq j - 1$ such that $(\mu_1 + 1)I + \mu_2 L^T L = \hat{L}\hat{L}^T$. This decomposition can be achieved by using Cholesky factorization. Thus solving equation (15) is equivalent to solving two systems of linear equations $\hat{L}z = X^T y + \mu_1(a^k - \mu_1^{-1}u^k) + \mu_2 L^T (b^k - \mu_2^{-1}v^k)$ and $\hat{L}^T \beta^{k+1} = z$. These two equations can be easily solved due to the special structure of \hat{L} .

The linear system (2.3) is very special for large p, small n problems in that $X^T X$ will be a low rank matrix with rank at most n. In combination of the special structure of matrix P mentioned above, we use preconditioned conjugate gradient algorithm (PCG) to solve (2.3).

The PCG algorithm [24] computes an approximate solution of the linear equations $H\mathbf{x} = \mathbf{g}$ using a preconditioner P, where both $H, P \in \mathbb{R}^{p \times p}$ are symmetric positive definite. For the linear equation (14), we use preconditioner $P = \mu_1 I + \mu_2 L^T L$ and the PCG algorithm converges in less than n steps. In our numerical implementation, we found that PCG converges in a few steps much smaller than n.

2.3. Split Bregman for FLSA (SBFLSA)

The fused Lasso signal approximator (FLSA) problem introduced by Friedman et al. corresponds to a special case of the standard fused Lasso with the predictor variables X being an identify matrix. Therefore, for FLSA, the primal problem minimizing β is simply

$$((\mu_1 + 1)I + \mu_2 L^T L)\beta^{k+1} = y + \mu_1(a^k - \mu_1^{-1}u^k) + \mu_2 L^T(b^k - \mu_2^{-1}v^k),$$
(15)

while other iterations stay the same.

As mentioned in the preceding section, matrix $(\mu_1 + 1)I + \mu_2 L^T L$ is a tridiagonal positive definite matrix, so (15) can be solved very efficiently, requiring only order of p operations. Therefore, we have a fast solver for SBFLSA using the split Bregman iteration in Algorithm 1.

2.4. Iterative algorithm for fused Lasso Support Vector Classifier (SBFLSVM)

Next we derive a split Bregman algorithm for the fused Lasso support vector classifier (FLSVM) introduced by [1]. FLSVM uses a hinge loss function [25] for two-label classification problems. It finds the optimal classification coefficients $(\hat{\beta}_0, \hat{\beta})$ that minimize

$$f(\beta_0, \beta) = \frac{1}{n} \sum_{i=1}^n (1 - y_i (\beta^T \mathbf{x}_i + \beta_0))_+ + \lambda_1 \|\beta\|_1 + \lambda_2 \|L\beta\|_1,$$
(16)

where $(u)_{+} = \max\{u, 0\}$ for any $u \in \mathbb{R}$ and L is the difference operator defined in (13).

Because the hinge loss function $(1 - t)_+$ is not differentiable, the primal problem involving β is now more difficult to solve. As a result, we will not directly apply Algorithm 1 to solve FLSVM. Instead, we introduce additional variables to deal with the nondifferentiability of the hinge loss.

Let Y be a diagonal matrix with its diagonal elements to be the vector y. The unconstrained problem in

(16) can be reformulated into an equivalent constrained optimization problem

$$\min_{\substack{\beta,\beta_0,a,b,c \ n}} \frac{1}{n} \sum_{i=1}^n (c_i)_+ + \lambda_1 \|a\|_1 + \lambda_2 \|b\|_1$$
s. t. $\beta = a$
 $L\beta = b$
 $1 - YX\beta - \beta_0 y = c,$
(17)

where $\mathbf{1}$ is an *n*-column vector of 1s.

The augmented Lagrangian function of (17) is

$$\mathcal{L}(\beta,\beta_0,a,b,c,u,v,w) = \frac{1}{n} \sum_{i=1}^n (c_i)_+ + \lambda_1 \|a\|_1 + \lambda_2 \|b\|_1 + \langle u,\beta - a \rangle + \langle v,L\beta - b \rangle + \langle w,\mathbf{1} - YX\beta - \beta_0 - c \rangle + \frac{\mu_1}{2} \|\beta - a\|_2^2 + \frac{\mu_2}{2} \|L\beta - b\|_2^2 + \frac{\mu_3}{2} \|\mathbf{1} - YX\beta - \beta_0 - c\|_2^2,$$

where u, v, w are dual variables corresponding to linear constraints $\beta = a$, $L\beta = b$, and $1 - YX\beta - \beta_0 y = c$ respectively. Positive reals μ_1, μ_2 and μ_3 are the penalty parameters for the violation of the linear constraints.

Similar to the derivation of Algorithm 1, we find the saddle point of \mathcal{L} by iteratively updating the primal and dual directions

$$\begin{cases} (\beta^{k+1}, \beta_0^{k+1}) = \arg\min_{\beta,\beta_0} \langle u^k, \beta - a^k \rangle + \langle v^k, L\beta - b^k \rangle + \langle w^k, \mathbf{1} - YX\beta - \beta_0 y - c^k \rangle \\ + \frac{\mu_1}{2} \|\beta - a^k\|_2^2 + \frac{\mu_2}{2} \|L\beta - b^k\|_2^2 + \frac{\mu_3}{2} \|\mathbf{1} - YX\beta - \beta_0 y - c^k\|_2^2, \\ a^{k+1} = \arg\min_a \lambda_1 \|a\|_1 + \langle u^k, \beta^{k+1} - a \rangle + \frac{\mu_1}{2} \|\beta^{k+1} - a\|_2^2, \\ b^{k+1} = \arg\min_b \lambda_2 \|b\|_1 + \langle v^k, L\beta^{k+1} - b \rangle + \frac{\mu_2}{2} \|L\beta^{k+1} - b\|_2^2, \\ c^{k+1} = \arg\min_c \frac{1}{n} \sum_{i=1}^n (c_i)_i + \langle w^k, \mathbf{1} - YX\beta^{k+1} - \beta_0^{k+1} y - c \rangle \\ + \frac{\mu_3}{2} \|\mathbf{1} - YX\beta^{k+1} - \beta_0^{k+1} y - c\|_2^2 \end{cases}$$
(18)
$$\frac{u^{k+1} = u^k + \delta_1(\beta^{k+1} - a^{k+1}), \\ v^{k+1} = v^k + \delta_3(\mathbf{1} - YX\beta^{k+1} - \beta_0^{k+1} y - c^{k+1}) \end{cases}$$

The update for $a^{k+1}, b^{k+1}, u^{k+1}, v^{k+1}, w^{k+1}$ are almost the same as the one in Algorithm 1, so we focus on the update for $(\beta^{k+1}, \beta_0^{k+1})$ and c^{k+1} . In Supplementary Information we show that PCG can still be applied to solve the updating of $(\beta^{k+1}, \beta_0^{k+1})$ with some modifications.

To update of c^{k+1} in 18, we use the following proposition, which is proven in the Supplementary Info.

Proposition 1. Let $s_{\lambda}(w) = \arg \min_{x \in \mathbb{R}} \lambda x_{+} + \frac{1}{2} ||x - w||_{2}^{2}$. Then

$$s_{\lambda}(w) = \begin{cases} w - \lambda, & w > \lambda, \\ 0, & 0 \le w \le \lambda, \\ w, & w < 0. \end{cases}$$
(19)

With Proposition 1, we can then update c^{k+1} in 18 according to

Corollary 1. $c^{k+1} = S_{\frac{1}{n\mu_3}} (1 - YX\beta^{k+1} - \beta_0^{k+1}y + \mu_3^{-1}w^k)$ is the solution of equation (??), where

$$\mathcal{S}_{\lambda}(w) = (s_{\lambda}(w_1), s_{\lambda}(w_2), \dots, s_{\lambda}(w_n)), \quad \forall w \in \mathbb{R}^n$$

with s_{λ} defined by (19).

Proof. The equation (??) is equivalent to

$$c^{k+1} = \arg\min_{c} \frac{1}{n\mu_3} \sum_{i=1}^{n} (c_i)_+ + \frac{1}{2} \|\mathbf{1} - YX\beta^{k+1} - \beta_0^{k+1}y - c + \mu_3^{-1}w^k\|_2^2.$$
(20)

Note that each element of c is independent of each other in (20), we can get the desired result by using Proposition 1.

In summary, we derive Algorithm 2 to solve (16).

Algorithm 2: Split Bregman method for FLSVM

$$\begin{aligned} \text{Initialize } \beta^{0}, \beta^{0}_{0}, a^{0}, b^{0}, c^{0}, u^{0}, v^{0}, \text{ and } w^{0}. \\ \textbf{repeat} \\ 1) \text{ Update } \beta^{k+1}, \beta^{k+1}_{0} \text{ by solving the linear equations:} \\ \begin{pmatrix} \mu_{1}I + \mu_{2}L^{T}L + \mu_{3}X^{T}Y^{2}X & \mu_{3}X^{T}Yy \\ \mu_{3}y^{T}YX & \mu_{3}y^{T}y \end{pmatrix} \begin{pmatrix} \beta^{k+1} \\ \beta^{k+1} \end{pmatrix} \\ = \mu_{1} \begin{pmatrix} a^{k} - \mu_{1}^{-1}u^{k} \\ 0 \end{pmatrix} + \mu_{2} \begin{pmatrix} L^{T} \\ 0 \end{pmatrix} (b^{k} - \mu_{2}^{-1}v^{k}) + \mu_{3} \begin{pmatrix} X^{T}Y \\ y^{T} \end{pmatrix} (\mathbf{1} - c^{k} + \mu_{3}^{-1}w^{k}) \\ 2) a^{k+1} = \mathcal{T}_{\mu_{1}^{-1}\lambda_{1}}(\beta^{k+1} + \mu_{1}^{-1}u^{k}) \\ 3) b^{k+1} = \mathcal{T}_{\mu_{2}^{-1}\lambda_{2}}(L\beta^{k+1} + \mu_{2}^{-1}v^{k}) \\ 4) c^{k+1} = \mathcal{S}_{\frac{1}{n\mu_{3}}}(\mathbf{1} - YX\beta^{k+1} - \beta^{k+1}_{0}y + \mu_{3}^{-1}w^{k}) \\ 5) u^{k+1} = u^{k} + \delta_{1}(L\beta^{k+1} - a^{k+1}) \\ 6) v^{k+1} = w^{k} + \delta_{2}(\beta^{k+1} - v^{k+1}) \\ \mathcal{T}) w^{k+1} = w^{k} + \delta_{3}(\mathbf{1} - YX\beta^{k+1} - \beta^{k+1}_{0}y - c^{k+1}) \end{aligned}$$

Convergence

The convergence property of Algorithm 2 is shown in the following theorem, which we prove in the Supplementary Info.

Theorem 2. Suppose there exists at least one solution β^* of (16). Assume $0 < \delta_1 \leq \mu_1, 0 < \delta_2 \leq \mu_2$ and $\lambda_1 > 0, \lambda_2 > 0$. Then the following property for Algorithm 2 holds:

$$\lim_{k \to \infty} \frac{1}{n} \sum_{i=1}^{n} (1 - y_i (\mathbf{x}_i^T \beta^k + \beta_0^k))_+ + \lambda_1 \|\beta^k\|_1 + \lambda_2 \|L\beta^k\|_1$$
$$= \frac{1}{n} \sum_{i=1}^{n} (1 - y_i (\mathbf{x}_i^T \beta^* + \beta_0^*))_+ + \lambda_1 \|\beta^*\|_1 + \lambda_2 \|L\beta^*\|_1.$$
(21)

Furthermore,

$$\lim_{k \to \infty} \|\beta^k - \beta^*\| = 0 \tag{22}$$

whenever (16) has a unique solution.

3. Experimental Results

Next we illustrate the efficiency of split Bregman method for fused Lasso using time trials on artificial data as well as real-world applications from genomics and proteomics. All our algorithms were implemented in Matlab, and compiled on a windows platform. Time trials were generated on an Intel Core 2 Duo desktop PC (E7500, 2.93GHz).

As the regression form of the fused Lasso procedures is more frequently used, we will thus focus on testing the performance of SBFLasso and SBFLSA. To evaluate the performance of SBFLasso, we compare it with SQOPT and CVX. SQOPT [5] is used in the original fused Lasso paper by Tibshirani et al. [1]. It is a two-phase active set algorithm, designed for quadratic programming problems with sparse linear constraints. CVX is a general convex optimization package [6]. SQOPT and CVX solve the fused Lasso by introducing additional variables and constraints to transform the nondifferentiable objective function into a smooth one. Both solvers are implemented in Matlab, and thus are directly comparable to our implementation. SQOPT allows warm start, so we will use it whenever possible. To evaluate the performance of SBFLSA for solving FLSA, we mainly compare it with the path algorithm proposed by Hoefling [9].

The stopping criterion of SBFLasso is specified as follows. Let $\Phi(\beta^k) = \frac{1}{2} ||X\beta^k - y||_2^2 + \lambda_1 ||\beta^k||_1 + \lambda_2 ||L\beta^k||_1$. According to Theorem 1, $\lim_{k\to\infty} \Phi(\beta^k) = \Phi(\beta^*)$. Therefore, we terminate SBFLasso when the relative change of the energy functional $\frac{1}{2} ||X\beta - y||_2^2 + \lambda_1 ||\beta||_1 + \lambda_2 ||L\beta||_1$ falls below certain threshold δ . We used $\delta = 10^{-5}$ in our simulation, i.e., we stop the Bregman iteration whenever

$$RelE := \frac{|\Phi(\beta^{k+1}) - \Phi(\beta^k)|}{\Phi(\beta^k)} \le 10^{-5}.$$
(23)

Note that the convergence of Algorithm 1 is guaranteed no matter what values of μ_1 and μ_2 are used as shown in Theorem 1. The speed of the algorithm can, however, be influenced by the choices of μ_1 and μ_2 as it would affect the number of iterations involved. In our implementation, we choose the parameter values using a pretrial procedure in which we test the convergence rate for a set of parameter values and identify the one that gives rise to the highest convergence rate. For regression problems, we always set $\mu_1 = \mu_2$ and select values from the set $\{0.2, 0.4, 0.6, 0.8, 1\} \times ||y||_2$. The parameter selecting procedure can certainly be further improved, but empirically we find it works well for all the problems we tested.

3.1. Artificial data

3.1.1. Solving fused Lasso

We generated Gaussian data with *n* observations and *p* predictors, with each pair of predictors $X_i, X_j (i \neq j)$ having the same population correlation ρ . The outcome values were generated by $Y = \sum_{j=1}^{p} \beta_j X_j + \epsilon$, where ϵ is the Gaussian noise with mean 0 and variance σ . The regression coefficient $\beta = (\beta_1, \ldots, \beta_p)$ is a sparse vector with the values of β_j are generated according to

$$\beta_i = \begin{cases} 2, & i = 1, 2..., 20, 121, 122, \dots, 125 \\ 3, & i = 41 \\ 1, & i = 71, 72, \dots, 85 \\ 0, & \text{else.} \end{cases}$$

The design of β is motivated by the fact that fused lasso are especially suitable for coefficients that are constant for an interval and change in jumps. An example plot of β of size p = 500 can be seen in Figure 1(a).

Table 1 shows the average CPU time for CVX, SQOPT and SBFLasso to solve the fused Lasso problems. SBFLasso consistently outperforms CVX in all cases we tested with a speedup of at least ten fold. Note that CVX fails to obtain results for large p problems due to out of memory errors. Although it has similar performance to SQOPT for small size problems ($p \sim 200$), SBFLasso is significantly faster than SQOPT for large p problems. For problems of n = 200, p = 20000, SBFLasso is able to obtain the optimal solutions within ~ 30 seconds, while it takes about 800 seconds for SQOPT to obtain the similar results. Overall, our algorithm is about twenty times faster than SQOPT for the large p problems.

To evaluate how the performance of SBFLasso scales with problem size, we plotted the CPU time that SBFLasso took to solve the fused Lasso problem as a function of p and n. Figure 2 shows such a curve, where CPU time is averaged over 500 runs with different parameters λ_1, λ_2 and different design matrix X. We note that the CPU times are roughly linear in both n and p.

A key to the success of SBFLasso is that we split the regularization terms $\|\beta\|_1$ and $\|L\beta\|_1$ and make the minimization problems separable. Due to the soft thresholding in the Bregman iteration, the solutions obtained by SBFLasso are naturally sparse as we can see from Figure 1(b). This is contrast to solutions obtained by CVX and SQOPT, because no thresholding steps are involved, solutions obtained by these two algorithms are not sparse, and sparseness can only be achieved through a thresholding step in the postprocessing.

3.1.2. Solving FLSA

Next we compare SBFLSA and the path algorithm (PATHFLSA) [9] for solving FLSA. PATHFLSA uses a fusion algorithm to solve FLSA, taking advantage of the special structure of the error term. It represents

		00	0 0	-	, (
		n=100	n=100	n=200	n=200	n=200	n=200
ρ	Method	p = 200	p=1000	p=2000	p = 5000	p=10000	p=20000
		time(sec)	time(sec)	time(sec)	time(sec)	time(sec)	time(sec)
	CVX	0.496	2.646	18.148	64.453	-	-
$\rho = 0$	SQOPT	0.0334	0.510	5.738	39.269	147.534	> 600
	SBFLasso	0.0366	0.155	1.488	5.845	12.724	28.441
	CVX	0.523	2.792	16.812	61.914	-	-
$\rho = 0.2$	SQOPT	0.0323	0.572	6.812	47.196	205.365	> 600
	SBFLasso	0.0352	0.323	2.831	9.716	18.249	34.061
	CVX	0.518	2.719	16.504	63.456	-	-
$\rho = 0.4$	SQOPT	0.0299	0.611	6.063	48.010	203.973	> 600
	SBFLasso	0.0338	0.265	2.803	8.897	24.680	26.990
	CVX	0.510	2.856	17.020	62.920	-	-
$\rho = 0.6$	SQOPT	0.0312	0.519	6.508	45.339	197.794	> 600
	SBFLasso	0.0286	0.143	2.190	8.947	20.586	36.157
	CVX	0.511	2.995	19.379	68.425	-	-
$\rho = 0.8$	SQOPT	0.0293	0.527	5.678	41.147	178.208	> 600
	SBFLasso	0.0190	0.221	1.426	6.446	15.505	41.614
-							

TABLE 1 Run times (CPU seconds) for fused lasso problems of various sizes p and n, different correlation ρ between the features. Methods are SQOPT, CVX and SBFLasso. The results are averaged over 100 runs (using 4 different predictor matrix X and 25 different values of regularization parameters λ_1, λ_2 (or s_1, s_2).



Fig 1: (a) The figure of coefficient β in 500 dimension; (b) The blue line is the solution derived by SBFLasso with $\lambda_1 = 16, \lambda_2 = 20$ and the red line is the original β in 500 dimension.



Fig 2: CPU times for SBFLasso for the same problem as in Table 1, for different values of n and p. In each case the times are averaged over 500 runs. (a) n is fixed and equals to 200; (b) p is fixed and equals to 5000.

the state of the art for solving the FLSA problem. We generate data according to $y = \beta + \epsilon$, where ϵ is the Gaussian noise with mean 0 and variance σ , and β is a sparse vector which has similar shape as the one shown in Figure 1(a) with more nonzero entries. We vary p from 10³ to 10⁶ and the results for each p are averaged over 10 runs.

Table 2 shows that the computational times of SBFLSA and PATHFLSA for solving the FLSA problems. We note that the performance of SBFLSA is similar to PATHFLSA in almost all cases we tested, and both algorithms significantly outperforms SQOPT with thousands of times faster for large p problems.

parameters	Method	$p = 10^{4}$	$p = 10^{5}$	$p = 10^{6}$
	SQOPT	106.97	> 5 hours	-
$\lambda_1 = 0.1, \lambda_2 = 0.8$	SBFLSA	0.053	0.754	8.681
	PATHFLSA	0.050	0.651	8.685
	SQOPT	107.74	> 5 hours	-
$\lambda_1 = 0.2, \lambda_2 = 1.0$	SBFLSA	0.053	0.820	8.263
	PATHFLSA	0.051	0.653	8.678
	SQOPT	108.12	> 5 hours	-
$\lambda_1 = 0.3, \lambda_2 = 1.2$	SBFLSA	0.053	0.798	9.289
	PATHFLSA	0.049	0.654	8.657
	SQOPT	106.13	> 5 hours	-
$\lambda_1 = 0.4, \lambda_2 = 1.5$	SBFLSA	0.053	0.806	9.892
	PATHFLSA	0.049	0.651	8.661

TABLE 2 Run times (CPU seconds) for an 1-dimensional FLSA problems of various sizes p. Methods are SQOPT, SBFLSA and path algorithm for FLSA(PATHFLSA). The results are averaged over 10 runs.

Although the performance of SBFLSA and PATHFLSA are similar for fixed λ_1 and λ_2 , PATHFLSA has an additional advantage of generating solutions for a path of the regularization parameters. However, because PATHFLSA works by fusing variables, a necessary condition for it to work is that the solution path has to be piece-wise linear when varying λ_2 . This condition is in general not true for both the fused Lasso and the generalized fused Lasso. As such, it cannot be applied to these cases.

3.2. Mass spectrometry data

Mass spectrometry (MS) holds great promise for biomarker identification, and genome wide metabolic and proteomic profiling. The protein mass spectroscopy application was used as a motivating example for fused Lasso in the paper by Tibshirani et al. [1]. Next we illustrate the efficiency of SBFLasso for solving the fused Lasso problem for mass spectrometry data. The data we use is taken from [26]. It consists of MS measurements of 95 normal samples and 121 samples taken from patients with ovarian cancer. The raw data contains a total of 368, 750 mass-to-charge ratio (m/z) sites.

We first preprocessed the data using the procedure described in [26], consisting of the following three steps: 1) re-sampling: Gaussian kernel reconstruction of the signal in order to have a set of *d*-dimensional vectors with equally spaced mass/charge values; 2) baseline correction: removes systematic artifacts, usually attributed to clusters of ionized matrix molecules hitting the detector during early portions of the experiment, or to detector overload; 3) normalization: corrects for differences in the total amount of protein desorbed and ionized from the sample plate. The average profiles from normal and cancer patients after preprocessing are shown in Figure 3.

TABLE 3 Run times (CPU seconds) for SBFLasso, SQOPT and CVX on MS data for different values of the regularization parameters λ_1 and λ_2 .

parameters	10-CV error	SBFLasso	SQOPT	CVX
$\lambda_1 = 2.0, \lambda_2 = 3.5$	6/216	2.9854	31.707	24.481
$\lambda_1 = 2.5, \lambda_2 = 4.5$	8/216	3.6612	30.310	23.456
$\lambda_1 = 3.0, \lambda_2 = 1.0$	6/216	3.2082	35.911	22.261
$\lambda_1 = 3.5, \lambda_2 = 2.5$	9/216	3.5080	32.094	21.130



Fig 3: (a) Protein mass spectroscopy data: average profiles from normal (blue) and cancer patients (red); (b) Estimated β from protein mass spectroscopy data with $\lambda_1 = 2, \lambda_2 = 3.5$ by CVX (blue) and SBFLasso (red).

We apply the fused Lasso (1) to the MS data to select features (m/z sites) that can be used to predict sample labels. For each sample, the response variable is either 1 or -1, and the predictor variable is a vector consisting of the intensity of p = 3000 sampled m/z sites. We used SBFLasso to solve the fused Lasso problem, and compared its performance to CVX and SQOPT. The results are summarized in Table 3, which shows the computational times spent by different solvers in a ten-fold cross-validation procedure for different parameters λ_1 and λ_2 . SBFLasso is consistently many times faster than CVX and SQOPT, with an approximately ten-fold speedup in almost all cases. The coefficients derived by SBFLasso and the other solvers are very similar (Figure 3b), but SBFLasso is able to achieve a sparser solution, and in addition a slightly lower objective function than CVX.

3.3. Comparative genomic hybridization (CGH) data

In tumor cells, mutations often cause a large DNA segment to be deleted or inserted in a chromosome, in a phenomena called copy number variation (CNV). Array CGH is a technique that is used to detect CNVs in a genome by labeling DNA from a test sample and normal reference sample differently using fluorophores and hybridizing to genomewide probes. The log ratio of the fluorescence intensity of the test DNA to the reference DNA is then calculated for each probe. A value greater than zero indicates a possible gain in DNA copies of the region around the probe, while a value less than zero suggests a possible loss. [3] demonstrated the efficiency of the fused lasso signal approximator (FLSA) for detecting CVNs using array CGH data. Next, we will show that SBFLSA is an efficient tool for solving the FLSA problem for array CGH data.

$Run\ times$	$(CPU \ seconds)$ for S	$BFLSA \ on \ CGH \ data$	for different values	of the regularizatio	n parameters	λ_1 and λ_2 .
	parameters	SBFLSA	PATHFLSA	SQOPT	CVX	
	$\lambda_1 = 0.10, \lambda_2 = 3.0$	0.007	0.006	0.7273	0.7124	
	$\lambda_1 = 0.12, \lambda_2 = 3.5$	0.007	0.005	0.6193	0.6451	
	$\lambda_1 = 0.15, \lambda_2 = 3.0$	0.007	0.006	0.6161	0.6604	
	$\lambda_1 = 0.18, \lambda_2 = 3.2$	0.006	0.005	0.6370	0.6244	

TABLE 4



Fig 4: Fused lasso applied to some GBM data. The data are shown in the left panel, and the solid red line in the right panel represents the inferred copy number $\hat{\beta}$ from SBFLSA. The gray line is for y = 0.

We used the glioblastoma multiforme (GBM) data from [27], which contains array CGN profiling of samples from primary GBMs, a particular malignant type of brain tumor. Table 4 shows the CPU times spent by SBFLSA to solve the FLSA problem for different regularization parameters λ_1 and λ_2 . We observe that our method is significantly faster than SQOPT and CVX, with a speed improvement of about 100 times. The performance of SBFLSA is also comparable to the path algorithm, which is specially designed, the state of the art for solving FLSA problems. Figure 4(b) plots the copy number variants detected by SBFLSA with $\lambda_1 = 0.10$ and $\lambda_2 = 3.5$, clearly showing the gain of DNA segments in two nearby chromosomal regions in GBM.

4. Discussion

Fused Lasso is an attractive framework for regression or classification problems with some natural ordering occurring in regression or classification coefficients. It exploits this naturally ordering by explicitly regularizing the differences between neighboring coefficients through an l_1 norm regularizer. Solving the fused

Lasso problem is, however, challenging because of the nondifferentiability of the objective function and the nonseparability of the variables involved in the nondifferentiable terms of the objective function. Existing solvers circumvent these difficulties by reformulating the fused Lasso problem into a smooth constrained convex optimization problem by introducing a large number of auxiliary variables and constraints, and as such, are only able to solve small or medium size fused Lasso problems.

We derived an iterative algorithm based on the split Bregman method to solve a class of fused Lasso problems, including SBFLasso for the standard fused Lasso, SBFLSA for the fused Lasso signal approximator, and SBFLSVM for fused Lasso support vector classifier, and proved their convergence properties. Preliminary experimental results for SBFLasso and SBFLSA show their efficiency for large scale problems, especially for problems with large p, small n, which occur in many real-world applications.

The iterative algorithm we propose is very easy to implement, involving only a few lines of code. It is also very general and can be adapted to solve a variety of fused Lasso problems with minor modifications as we have shown. In this aspect, it is very different from the path algorithm, which is specially designed for FLSA and requires significant amount of domain specific knowledge. Because of its simplicity and generality, we expect the split Bregman iterative algorithm would find its usage in a wide range of other ℓ_1 related regularization problems.

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Appendix

A.1. Convergence analysis of Algorithm 1

We use some similar ideas from Cai et al. [15] to prove Theorem 1. Different from the case of Cai et al. [15], we do not require $V(\beta)$ to be differentiable, and treat the nondifferentiability of $V(\beta)$ explicitly by using its subgradient vector $h \in \partial V(\beta)$, see the proof for details.

Proof of Theorem 1: Since all the subproblems involved in (8) are convex, the first order optimality condition of the Algorithm 1 gives

$$\begin{cases} 0 = h^{k+1} + u^k + L^T v^k + \mu_1(\beta^{k+1} - a^k) + \mu_2 L^T (L\beta^{k+1} - b^k), \\ \lambda_1 p^{k+1} - u^k + \mu_1(a^{k+1} - \beta^{k+1}) = 0, \\ \lambda_1 q^{k+1} - v^k + \mu_2(b^{k+1} - L\beta^{k+1}) = 0, \\ u^{k+1} = u^k + \delta_1(\beta^{k+1} - a^{k+1}), \\ v^{k+1} = v^k + \delta_2 (L\beta^{k+1} - b^{k+1}), \end{cases}$$

$$(24)$$

where $h^{k+1} \in \partial V(\beta^{k+1}), p^{k+1} \in \partial ||a^{k+1}||_1$ and $q^{k+1} \in \partial ||b^{k+1}||_1$.

Since β^* is a solution of (2), by the first order optimality condition, there exist h^*, p^*, q^* such that

$$h^* + \lambda_1 p^* + \lambda_2 L^T q^* = 0 \tag{25}$$

where $h^* \in \partial V(\beta), p^* \in \partial \|\beta^*\|_1, q^* \in \partial \|b^*\|_1$ with $b^* = L\beta^*$. Introducing new variables $a^* = \beta^*, u^* = \lambda_1 p^*, v^* = \lambda_2 q^*$, we can formulate (25) as

$$\begin{cases} 0 = h^* + u^* + L^T v^* + \mu_1(\beta^* - a^*) + \mu_2 L^T (L\beta^* - b^*), & \text{with} \quad h^* \in \partial V(\beta) \\ \lambda_1 p^* - u^* + \mu_1(a^* - \beta^*) = 0, & \text{with} \quad p^* \in \partial ||a^*||_1, \\ \lambda_1 q^* - v^* + \mu_2(b^* - L\beta^*) = 0, & \text{with} \quad q^* \in \partial ||b^*||_1, \\ u^* = u^* + \delta_1(\beta^* - a^*), \\ v^* = v^* + \delta_2(L\beta^* - b^*). \end{cases}$$
(26)

Comparing (26) with (24), we can see that $\beta^*, a^*, b^*, u^*, v^*$ is a fix point of Algorithm 1. Denote the errors by

$$\beta_e^k = \beta^k - \beta^*, a_e^k = a^k - a^*, b_e^k = b^k - b^*, u_e^k = u^k - u^* \text{ and } v_e^k = v^k - v^*.$$

Subtracting the first equation of (24) by the first equation of (26), we obtain

$$0 = h^{k+1} - h^* + u_e^k + L^T v_e^k + \mu_1(\beta_e^{k+1} - a_e^k) + \mu_2 L^T (L\beta_e^{k+1} - b_e^k)$$

Taking the inner product of the left and right hand sides with respect to β_e^{k+1} , we have

$$0 = \langle h^{k+1} - h^*, \beta^{k+1} - \beta^* \rangle + \langle u_e^k, \beta_e^{k+1} \rangle + \langle v_e^k, L\beta_e^{k+1} \rangle + \mu_1 \|\beta_e^{k+1}\|_2^2 - \mu_1 \langle a_e^k, \beta_e^{k+1} \rangle + \mu_2 \|L\beta_e^{k+1}\|_2^2 - \mu_2 \langle b_e^k, L\beta_e^{k+1} \rangle$$
(27)

Similarly, we can get

$$\lambda_1 \langle p^{k+1} - p^*, a^{k+1} - a^* \rangle + \mu_1 \| a_e^{k+1} \|_2^2 - \mu_1 \langle a_e^{k+1}, \beta_e^{k+1} \rangle - \langle u_e^k, a_e^{k+1} \rangle = 0,$$
(28)

$$\lambda_2 \langle q^{k+1} - q^*, b^{k+1} - b^* \rangle + \mu_2 \| b_e^{k+1} \|_2^2 - \mu_2 \langle b_e^{k+1}, L\beta_e^{k+1} \rangle - \langle v_e^k, b_e^{k+1} \rangle = 0.$$
⁽²⁹⁾

Summing (27), (28) and (29) together, we get

$$\langle h^{k+1} - h^*, \beta^{k+1} - \beta^* \rangle + \lambda_1 \langle p^{k+1} - p^*, a^{k+1} - a^* \rangle + \lambda_2 \langle q^{k+1} - q^*, b^{k+1} - b^* \rangle$$

$$+ \mu_1 (\|\beta_e^{k+1}\|_2^2 + \|a_e^{k+1}\|_2^2 - \langle \beta_e^{k+1}, a_e^k + a_e^{k+1} \rangle) + \mu_2 (\|L\beta_e^{k+1}\|_2^2 + \|b_e^{k+1}\|_2^2$$

$$- \langle L\beta_e^{k+1}, b_e^k + b_e^{k+1} \rangle) + \langle u_e^k, \beta_e^{k+1} - a_e^{k+1} \rangle + \langle v_e^k, L\beta_e^{k+1} - b_e^{k+1} \rangle = 0$$

$$(30)$$

Furthermore, by subtracting the fourth equation of (24) by the one of (26), we have

$$u_e^{k+1} = u_e^k + \delta_1(\beta_e^{k+1} - a_e^{k+1}).$$

Taking square of both sides of the above equation implies

$$\langle u_e^k, \beta_e^{k+1} - a_e^{k+1} \rangle = \frac{1}{2\delta_1} (\|u_e^{k+1}\|_2^2 - \|u_e^k\|_2^2) - \frac{\delta_1}{2} \|\beta_e^{k+1} - a_e^{k+1}\|_2^2.$$
(31)

Similarly, we have

$$\langle v_e^k, L\beta_e^{k+1} - b_e^{k+1} \rangle = \frac{1}{2\delta_2} (\|v_e^{k+1}\|_2^2 - \|v_e^k\|_2^2) - \frac{\delta_2}{2} \|L\beta_e^{k+1} - b_e^{k+1}\|_2^2.$$
(32)

Substituting (31) and (32) into (30) yields

$$\frac{1}{2\delta_{1}}(\|u_{e}^{k}\|_{2}^{2} - \|u_{e}^{k+1}\|_{2}^{2}) + \frac{1}{2\delta_{2}}(\|v_{e}^{k}\|_{2}^{2} - \|v_{e}^{k+1}\|_{2}^{2}) \\
= \langle h^{k+1} - h^{*}, \beta^{k+1} - \beta^{*} \rangle + \lambda_{1} \langle p^{k+1} - p^{*}, a^{k+1} - a^{*} \rangle + \lambda_{2} \langle q^{k+1} - q^{*}, b^{k+1} - b^{*} \rangle \\
+ \mu_{1}(\|\beta_{e}^{k+1}\|_{2}^{2} + \|a_{e}^{k+1}\|_{2}^{2} - \langle \beta_{e}^{k+1}, a_{e}^{k} + a_{e}^{k+1} \rangle - \frac{\delta_{1}}{2\mu_{1}} \|\beta_{e}^{k+1} - a_{e}^{k+1}\|_{2}^{2}) \\
+ \mu_{2}(\|L\beta_{e}^{k+1}\|_{2}^{2} + \|b_{e}^{k+1}\|_{2}^{2} - \langle L\beta_{e}^{k+1}, b_{e}^{k} + b_{e}^{k+1} \rangle - \frac{\delta_{2}}{2\mu_{2}} \|L\beta_{e}^{k+1} - b_{e}^{k+1}\|_{2}^{2}) \tag{33}$$

Note that for any $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^p$, we have

$$\|\mathbf{x}\|_{2}^{2} \pm \langle \mathbf{x}, \mathbf{y} + \mathbf{z} \rangle + \|\mathbf{y}\|_{2}^{2} = \frac{1}{2} \|\mathbf{x} \pm \mathbf{y}\|_{2}^{2} + \frac{1}{2} \|\mathbf{x} \pm \mathbf{z}\|_{2}^{2} + \frac{1}{2} (\|\mathbf{y}\|_{2}^{2} - \|\mathbf{z}\|_{2}^{2}).$$
(34)

Using this elementary equation, (33) can be transformed to

$$\begin{aligned} &\frac{1}{2\delta_1} (\|u_e^k\|_2^2 - \|u_e^{k+1}\|_2^2) + \frac{1}{2\delta_2} (\|v_e^k\|_2^2 - \|v_e^{k+1}\|_2^2) \\ &= \langle h^{k+1} - h^*, \beta^{k+1} - \beta^* \rangle + \lambda_1 \langle p^{k+1} - p^*, a^{k+1} - a^* \rangle + \lambda_2 \langle q^{k+1} - q^*, b^{k+1} - b^* \rangle \\ &+ \frac{\mu_1}{2} \left(\|\beta_e^{k+1} - a_e^k\|_2^2 + \|a_e^{k+1}\|_2^2 - \|a_e^k\|_2^2 + \frac{\mu_1 - \delta_1}{\mu_1}\|\beta_e^{k+1} - a_e^{k+1}\|_2^2 \right) \\ &+ \frac{\mu_2}{2} \left(\|L\beta_e^{k+1} - b_e^k\|_2^2 + \|b_e^{k+1}\|_2^2 - \|b_e^k\|_2^2 + \frac{\mu_2 - \delta_2}{\mu_2}\|L\beta_e^{k+1} - b_e^{k+1}\|_2^2 \right) \end{aligned}$$

Summing the above equation from k = 0 to k = K yields

$$\frac{1}{2\delta_{1}}(\|u_{e}^{0}\|_{2}^{2} - \|u_{e}^{K+1}\|_{2}^{2}) + \frac{1}{2\delta_{2}}(\|v_{e}^{0}\|_{2}^{2} - \|v_{e}^{K+1}\|_{2}^{2}) \\
+ \frac{\mu_{1}}{2}(\|a_{e}^{0}\|_{2}^{2} - \|a_{e}^{K+1}\|_{2}^{2}) + \frac{\mu_{2}}{2}(\|b_{e}^{0}\|_{2}^{2} - \|b_{e}^{K+1}\|_{2}^{2}) \\
= \sum_{k=0}^{K} \langle h^{k+1} - h^{*}, \beta^{k+1} - \beta^{*} \rangle + \lambda_{1} \sum_{k=0}^{K} \langle p^{k+1} - p^{*}, a^{k+1} - a^{*} \rangle \\
+ \lambda_{2} \sum_{k=0}^{K} \langle q^{k+1} - q^{*}, b^{k+1} - b^{*} \rangle + \frac{\mu_{1}}{2} \sum_{k=0}^{K} \|\beta_{e}^{k+1} - a_{e}^{k}\|_{2}^{2} + \frac{\mu_{1} - \delta_{1}}{\mu_{1}} \sum_{k=0}^{K} \|\beta_{e}^{k+1} - a_{e}^{k+1}\|_{2}^{2} \\
+ \frac{\mu_{2}}{2} \sum_{k=0}^{K} \|L\beta_{e}^{k+1} - b_{e}^{k}\|_{2}^{2} + \frac{\mu_{2} - \delta_{2}}{\mu_{2}} \sum_{k=0}^{K} \|L\beta_{e}^{k+1} - b_{e}^{k+1}\|_{2}^{2} \tag{35}$$

The fact that $h^{k+1} \in \partial V(\beta^{k+1}), h^* \in \partial V(\beta^*)$ and $V(\beta)$ is convex implies

$$\langle h^{k+1} - h^*, \beta^{k+1} - \beta^* \rangle = V(\beta^{k+1}) - V(\beta^*) - \langle h^*, \beta^{k+1} - \beta^* \rangle + V(\beta^*) - V(\beta^{k+1}) - \langle h^{k+1}, \beta^{k+1} - \beta^* \rangle \geq 0$$
(36)

by the definition of subgradient. Similarly, $\langle p^{k+1} - p^*, a^{k+1} - a^* \rangle \ge 0, \langle q^{k+1} - q^*, b^{k+1} - b^* \rangle \ge 0$. Together with the fact that $0 < \delta_1 \le \mu_1$ and $0 < \delta_2 \le \mu_2$, all terms involved in (35) are nonnegative. Therefore,

$$\sum_{k=0}^{\infty} \langle h^{k+1} - h^*, \beta^{k+1} - \beta^* \rangle \le \frac{1}{2\delta_1} \|u_e^0\|_2^2 + \frac{1}{2\delta_2} \|v_e^0\|_2^2 + \frac{\mu_1}{2} \|a_e^0\|_2^2 + \frac{\mu_2}{2} \|b_e^0\|_2^2$$

which leads to

$$\lim_{k \to \infty} \langle h^k - h^*, \beta^k - \beta^* \rangle = 0$$

Together with (36) leads to

$$\lim_{k \to \infty} V(\beta^k) - V(\beta^*) - \langle h^*, \beta^k - \beta^* \rangle = 0.$$
(37)

Similarly, we can prove

$$\lambda_1 \lim_{k \to \infty} \|a^k\|_1 - \|a^*\|_1 - \langle a^k - a^*, p^* \rangle = 0,$$
(38)

$$\lambda_2 \lim_{k \to \infty} \|b^k\|_1 - \|b^*\|_1 - \langle b^k - b^*, q^* \rangle = 0,$$
(39)

$$\lim_{k \to \infty} \|\beta^k - a^k\|_2 = 0 \quad \text{and} \quad \lim_{k \to \infty} \|L\beta^k - b^k\|_2 = 0.$$
(40)

Since $\|\cdot\|_1$ is continuous, by (38),(39) and (40), we obtain

$$\lambda_1 \lim_{k \to \infty} \|\beta^k\|_1 - \|\beta^*\|_1 - \langle\beta^k - \beta^*, p^*\rangle = 0,$$
(41)

$$\lambda_2 \lim_{k \to \infty} \|L\beta^k\|_1 - \|L\beta^*\|_1 - \langle L\beta^k - L\beta^*, q^* \rangle = 0.$$
(42)

Summing (37), (41) and (42) yields

$$\lim_{k \to \infty} V(\beta^k) + \lambda_1 \|\beta^k\|_1 + \lambda_2 \|L\beta^k\|_1 - (V(\beta^*) + \lambda_1 \|\beta^*\|_1 + \lambda_2 \|L\beta^*\|_1) + \langle \beta^k - \beta^*, h^* + p^* + L^T q^* \rangle = 0$$

This together with (25) proves

$$\lim_{k \to \infty} V(\beta^k) + \lambda_1 \|\beta^k\|_1 + \lambda_2 \|L\beta^k\|_1 = V(\beta^*) + \lambda_1 \|\beta^*\|_1 + \lambda_2 \|L\beta^*\|_1.$$
(43)

Next, we prove that

$$\lim_{k \to \infty} \|\beta^k - \beta^*\|_2 = 0 \tag{44}$$

whenever (2) has a unique solution.

It is proved by contradiction. Let $\Phi(\beta) = V(\beta) + \lambda_1 \|\beta\|_1 + \lambda_2 \|L\beta\|_1$. Then $\Phi(\beta)$ is a convex, lower continuous function. Since β^* is the unique minimizer, we have $\Phi(\beta) > \Phi(\beta^*)$ for all $\beta \neq \beta^*$. If (44) does not hold, there exists a subsequence β^{k_i} such that $\|\beta^{k_i} - \beta^*\| > \epsilon$ for some $\epsilon > 0$ and for all *i*. Then $\Phi(\beta^{k_i}) > \min\{\Phi(\beta) : \|\beta - \beta^*\|_2 = \epsilon\}$. Indeed, let γ be the intersection of the sphere $\{\beta : \|\beta - \beta^*\|_2 = \epsilon\}$ and line segment from β^* to β^{k_i} , then there exists a positive number $t \in (0, 1)$ such that $\gamma = t\beta^* + (1 - t)\beta^{k_i}$. By the convexity of Φ and the definition of β^* , we have

$$\begin{aligned} \Phi(\beta^{k_i}) &> t\Phi(\beta^*) + (1-t)\Phi(\beta^{k_i}) \ge \Phi(t\beta^* + (1-t)\beta^{k_i}) \\ &= \Phi(\gamma) \ge \min\{\Phi(\beta) : \|\beta - \beta^*\|_2 = \epsilon\}. \end{aligned}$$

Denote $\tilde{\beta} = \arg\min\{\Phi(\beta) : \|\beta - \beta^*\|_2 = \epsilon\}$. By applying (43), we have

$$\Phi(\beta^*) = \lim_{i \to \infty\infty} \Phi(\beta^{k_i}) \ge \Phi(\tilde{\beta}) > \Phi(\beta^*),$$

which is a contradiction.

A.2. Convergence analysis of Algorithm 2

Now we give the proof of Theorem 2. The main idea is the same as the one in [15]. However, due to the extra bias term β_0 and the hinge loss, the terms involved in our proof are more complicated.

Since all the subproblems involved in (18) are convex, the first order optimality condition gives

$$\begin{pmatrix} \begin{pmatrix} \mu_{1}I + \mu_{2}L^{T}L + \mu_{3}X^{T}Y^{2}X & \mu_{3}X^{T}Yy \\ \mu_{3}y^{T}YX & \mu_{3}y^{T}y \end{pmatrix} \begin{pmatrix} \beta^{k+1} \\ \beta^{k+1}_{0} \end{pmatrix} \\ = \mu_{1} \begin{pmatrix} a^{k} - \mu_{1}^{-1}u^{k} \\ 0 \end{pmatrix} + \mu_{2} \begin{pmatrix} L^{T} \\ 0 \end{pmatrix} (b^{k} - \mu_{2}^{-1}v^{k}) + \mu_{3} \begin{pmatrix} X^{T}Y \\ y^{T} \end{pmatrix} (\mathbf{1} - c^{k} + \mu_{3}^{-1}w^{k}) \\ \lambda_{1}p^{k+1} - u^{k} + \mu_{1}(a^{k+1} - \beta^{k+1}) = 0, \\ \lambda_{2}q^{k+1} - v^{k} + \mu_{2}(b^{k+1} - L\beta^{k+1}) = 0, \\ \frac{1}{n}s^{k+1} - w^{k} + \mu_{3}(c^{k+1} + YX\beta^{k+1} + \beta^{k+1}_{0}y - \mathbf{1}) = 0, \\ u^{k+1} = u^{k} + \delta_{1}(\beta^{k+1} - a^{k+1}), \\ v^{k+1} = v^{k} + \delta_{2}(L\beta^{k+1} - b^{k+1}), \\ w^{k+1} = w^{k} + \delta_{3}(\mathbf{1} - YX\beta^{k+1} - \beta^{k+1}_{0}y - c^{k+1}), \end{pmatrix}$$

$$(45)$$

where $p^{k+1} \in \partial ||a^{k+1}||_1, q^{k+1} \in \partial ||b^{k+1}||_1$ and $s^{k+1} \in \partial ||c^{k+1}||_1$. This simple observation will be used in our proof for the convergence of SBFLSVM.

Proof of Theorem 2. Let (β^*, β_0^*) be an arbitrary minimizer of (16). By the first order optimality condition, there exist p^*, q^* and s^* such that

$$\begin{cases} -\frac{1}{n}X^T Y s^* + \lambda_1 p^* + \lambda_2 L^T q^* = 0, \\ y^T s^* = 0, \end{cases}$$
(46)

where $s_i^* \in \partial(c_i^*)_+$ with $c_i^* = 1 - y_i(\mathbf{x}_i^T \beta^* + \beta_0^*), i = 1, ..., n, p^* \in \partial \|\beta^*\|_1, q^* \in \partial \|b^*\|_1$ with $b^* = L\beta^*$. Introducing new variables $a^* = \beta^*, u^* = \lambda_1 p^*, v^* = \lambda_2 q^*$ and $w^* = \frac{1}{n} s^*$, we can formulate (46) as

$$\begin{cases} \begin{pmatrix} \mu_{1}I + \mu_{2}L^{T}L + \mu_{3}X^{T}Y^{2}X & \mu_{3}X^{T}Yy \\ \mu_{3}y^{T}YX & \mu_{3}y^{T}y \end{pmatrix} \begin{pmatrix} \beta^{*} \\ \beta^{*}_{0} \end{pmatrix} \\ = \mu_{1} \begin{pmatrix} a^{*} - \mu_{1}^{-1}u^{*} \\ 0 \end{pmatrix} + \mu_{2} \begin{pmatrix} L^{T} \\ 0 \end{pmatrix} (b^{*} - \mu_{2}^{-1}v^{*}) + \mu_{3} \begin{pmatrix} X^{T}Y \\ y^{T} \end{pmatrix} (\mathbf{1} - c^{*} + \mu_{3}^{-1}w^{*}) \\ \lambda_{1}p^{*} - u^{*} + \mu_{1}(a^{*} - \beta^{*}) = 0, \quad \text{with} \quad p^{*} \in \partial ||a^{*}||_{1} \\ \lambda_{2}q^{*} - v^{*} + \mu_{2}(b^{*} - L\beta^{*}) = 0, \quad \text{with} \quad q^{*} \in \partial ||b^{*}||_{1} \\ \frac{1}{n}s^{*} - w^{*} + \mu_{3}(c^{*} + YX\beta^{*} + \beta^{*}_{0}y - \mathbf{1}) = 0, \quad \text{with} \quad s^{*} \in \partial (\sum_{i=1}^{n}(c_{i})_{+}) \\ u^{*} = u^{*} + \delta_{1}(\beta^{*} - a^{*}), \\ v^{*} = v^{*} + \delta_{3}(\mathbf{1} - YX\beta^{*} - \beta^{*}_{0}y - c^{*}). \end{cases}$$

$$(47)$$

Therefore, $\beta^*, \beta_0^*, a^*, b^*, c^*, u^*, v^*, w^*$ is a fixed point of (45). Denote the errors by

$$\beta_e^k = \beta^k - \beta^*, \beta_{0e}^k = \beta_0^k - \beta_0^*, a_e^k = a^k - a^*, b_e^k = b^k - b^*,$$
$$c_e^k = c^k - c^*, u_e^k = u^k - u^*, v_e^k = v^k - v^* \text{ and } w_e^k = w^k - w^*$$

Subtracting the first equation of (45) by the first equation of (47), we obtain

$$\begin{pmatrix} \mu_1 I + \mu_2 L^T L + \mu_3 X^T Y^2 X & \mu_3 X^T Y y \\ \mu_3 y^T Y X & \mu_3 y^T y \end{pmatrix} \begin{pmatrix} \beta_e^{k+1} \\ \beta_e^{k+1} \end{pmatrix}$$

= $\mu_1 \begin{pmatrix} a_e^k - \mu_1^{-1} u_e^k \\ 0 \end{pmatrix} + \mu_2 \begin{pmatrix} L^T \\ 0 \end{pmatrix} (b_e^k - \mu_2^{-1} v_e^k) + \mu_3 \begin{pmatrix} X^T Y \\ y^T \end{pmatrix} (-c_e^k + \mu_3^{-1} w_e^k)$
= 18

Taking the inner product of the left and right hand sides with respect to $((\beta_e^{k+1})^T, \beta_{0e}^{k+1})^T$, we have

$$\begin{array}{ll} \langle (\mu_{1}I + \mu_{2}L^{T}L + \mu_{3}X^{T}Y^{2}X)\beta_{e}^{k+1} + \mu_{3}X^{T}Yy\beta_{0e}^{k+1}, \beta_{e}^{k+1}\rangle + \mu_{3}\langle YX\beta_{e}^{k+1} + y\beta_{0e}^{k+1}, y\beta_{0e}^{k+1}\rangle \\ = & \mu_{1}\langle a_{e}^{k}, \beta_{e}^{k+1}\rangle - \langle u_{e}^{k}, \beta_{e}^{k+1}\rangle + \mu_{2}\langle b_{e}^{k}, L\beta_{e}^{k+1}\rangle - \langle v_{e}^{k}, L\beta_{e}^{k+1}\rangle \\ & -\mu_{3}\langle c_{e}^{k}, YX\beta_{e}^{k+1}\rangle + \langle w_{e}^{k}, YX\beta_{e}^{k+1}\rangle - \mu_{3}\langle c_{e}^{k}, y\beta_{0e}^{k+1}\rangle + \langle w_{e}^{k}, y\beta_{0e}^{k+1}\rangle. \end{array}$$

$$\tag{48}$$

The same manipulations applied to the second (third, fourth) of equation (45) and the second (third, fourth) of equation (47) lead to

$$\lambda_1 \langle p^{k+1} - p^*, a^{k+1} - a^* \rangle + \mu_1 \|a_e^{k+1}\|_2^2 - \langle u_e^k, a_e^{k+1} \rangle - \mu_1 \langle \beta_e^{k+1}, a_e^{k+1} \rangle = 0.$$
(49)

$$\lambda_2 \langle q^{k+1} - q^*, b^{k+1} - b^* \rangle + \mu_2 \| b_e^{k+1} \|_2^2 - \langle v_e^k, b_e^{k+1} \rangle - \mu_2 \langle L \beta_e^{k+1}, b_e^{k+1} \rangle = 0.$$
(50)

$$\frac{1}{n}\langle s^{k+1} - s^*, c^{k+1} - c^* \rangle + \mu_3 \|c_e^{k+1}\|_2^2 - \langle w_e^k, c_e^{k+1} \rangle + \mu_3 \langle YX\beta_e^{k+1} + \beta_{0e}^{k+1}y, c_e^{k+1} \rangle = 0.$$
(51)

By summing equations (48), (49), (50) and (51), we get

$$\begin{split} \lambda_1 \langle p^{k+1} - p^*, a^{k+1} - a^* \rangle + \lambda_2 \langle q^{k+1} - q^*, b^{k+1} - b^* \rangle + \frac{1}{n} \langle s^{k+1} - s^*, c^{k+1} - c^* \rangle \\ + \mu_1 (\|\beta_e^{k+1}\|_2^2 - \langle \beta_e^{k+1}, a_e^{k+1} + a_e^k \rangle + \|a_e^{k+1}\|_2^2) \\ + \mu_2 (\|L\beta_e^{k+1}\|_2^2 - \langle b_e^{k+1} + b_e^k, L\beta_e^{k+1} \rangle + \|b_e^{k+1}\|_2^2) \\ + \mu_3 (\|YX\beta_e^{k+1} + y\beta_{0e}^{k+1}\|_2^2 + \mu_3 \langle YX\beta_e^{k+1} + y\beta_{0e}^{k+1}, c_e^{k+1} + c_e^k \rangle + \|c_e^{k+1}\|_2^2) \\ + \langle u_e^k, \beta_e^{k+1} - a_e^{k+1} \rangle + \langle v_e^k, L\beta_e^{k+1} - b_e^{k+1} \rangle - \langle w_e^k, YX\beta_e^{k+1} + y\beta_{0e}^{k+1} + c_e^{k+1} \rangle = 0. \end{split}$$
(52)

Furthermore, subtracting the fifth equation of (45) by the fifth equation of (47), we have

$$u_e^{k+1} = u_e^k + \delta_1(\beta_e^{k+1} - a_e^{k+1}).$$

which leads to

$$\langle u_e^k, \beta_e^{k+1} - a_e^{k+1} \rangle = \frac{1}{2\delta_1} (\|u_e^{k+1}\|_2^2 - \|u_e^k\|_2^2) - \frac{\delta_1}{2} \|\beta_e^{k+1} - a_e^{k+1}\|_2^2.$$
(53)

Similarly, we can get

$$\langle v_e^k, L\beta_e^{k+1} - b_e^{k+1} \rangle = \frac{1}{2\delta_2} (\|v_e^{k+1}\|_2^2 - \|v_e^k\|_2^2) - \frac{\delta_2}{2} \|L\beta_e^{k+1} - b_e^{k+1}\|_2^2$$
(54)

and

$$\langle w_e^k, YX\beta_e^{k+1} + \beta_{0e}^{k+1}y + c_e^{k+1} \rangle$$

$$= -\frac{1}{2\delta_3} (\|w_e^{k+1}\|_2^2 - \|w_e^k\|_2^2) + \frac{\delta_3}{2} \|YX\beta_e^{k+1} + \beta_{0e}^{k+1}y + c_e^{k+1}\|_2^2.$$
(55)

Substituting (53), (54) and (55) into (52) yields

$$\frac{1}{2\delta_{1}}(\|u_{e}^{k}\|_{2}^{2} - \|u_{e}^{k+1}\|_{2}^{2}) + \frac{1}{2\delta_{2}}(\|v_{e}^{k}\|_{2}^{2} - \|v_{e}^{k+1}\|_{2}^{2}) + \frac{1}{2\delta_{3}}(\|w_{e}^{k}\|_{2}^{2} - \|w_{e}^{k+1}\|_{2}^{2})$$

$$= \lambda_{1}\langle p^{k+1} - p^{*}, a^{k+1} - a^{*}\rangle + \lambda_{2}\langle q^{k+1} - q^{*}, b^{k+1} - b^{*}\rangle + \frac{1}{n}\langle s^{k+1} - s^{*}, c^{k+1} - c^{*}\rangle + \mu_{1}\left(\|\beta_{e}^{k+1}\|_{2}^{2} - \langle\beta_{e}^{k+1}, a_{e}^{k+1} + a_{e}^{k}\rangle + \|a_{e}^{k+1}\|_{2}^{2} - \frac{\delta_{1}}{2\mu_{1}}\|\beta_{e}^{k+1} - a_{e}^{k+1}\|_{2}^{2}\right) + \mu_{2}\left(\|L\beta_{e}^{k+1}\|_{2}^{2} - \langle L\beta_{e}^{k+1}, b_{e}^{k+1} + b_{e}^{k}\rangle + \|b_{e}^{k+1}\|_{2}^{2} - \frac{\delta_{2}}{2\mu_{2}}\|L\beta_{e}^{k+1} - b_{e}^{k+1}\|_{2}^{2}\right) + \mu_{3}\left(\|YX\beta_{e}^{k+1} + y\beta_{0e}^{k+1} + y\beta_{0e}^{k+1}\|_{2}^{2} + \langle YX\beta_{e}^{k+1} + y\beta_{0e}^{k+1}, c_{e}^{k+1} + c_{e}^{k}\rangle + \|c_{e}^{k+1}\|_{2}^{2} - \frac{\delta_{3}}{2\mu_{3}}\|YX\beta_{e}^{k+1} + \beta_{0e}^{k+1}y + c_{e}^{k+1}\|_{2}^{2}\right).$$

$$(56)$$

Using the elementary equality (34), (56) can be transformed to

$$\begin{split} &\frac{1}{2\delta_1}(\|u_e^k\|_2^2 - \|u_e^{k+1}\|_2^2) + \frac{1}{2\delta_2}(\|v_e^k\|_2^2 - \|v_e^{k+1}\|_2^2) + \frac{1}{2\delta_3}(\|w_e^k\|_2^2 - \|w_e^{k+1}\|_2^2) \\ &= \lambda_1 \langle p^{k+1} - p^*, a^{k+1} - a^* \rangle + \lambda_2 \langle q^{k+1} - q^*, b^{k+1} - b^* \rangle + \frac{1}{n} \langle s^{k+1} - s^*, c^{k+1} - c^* \rangle \\ &+ \frac{\mu_1}{2} \left(\|\beta_e^{k+1} - a_e^k\|_2^2 + \|a_e^{k+1}\|_2^2 - \|a_e^k\|_2^2 + \frac{\mu_1 - \delta_1}{\mu_1}\|\beta_e^{k+1} - a_e^{k+1}\|_2^2 \right) \\ &+ \frac{\mu_2}{2} \left(\|L\beta_e^{k+1} - b_e^k\|_2^2 + \|b_e^{k+1}\|_2^2 - \|b_e^k\|_2^2 + \frac{\mu_2 - \delta_2}{\mu_2}\|L\beta_e^{k+1} - b_e^{k+1}\|_2^2 \right) \\ &+ \frac{\mu_3}{2} \left(\|YX\beta_e^{k+1} + y\beta_{0e}^{k+1} + c_e^k\|_2^2 + \|c_e^{k+1}\|_2^2 - \|c_e^k\|_2^2 \\ &+ \frac{\mu_3 - \delta_3}{\mu_3}\|YX\beta_e^{k+1} + \beta_{0e}^{k+1}y + c_e^{k+1}\|_2^2 \right). \end{split}$$

(57)

Summing the above equation from k = 0 to k = K yields

$$\begin{aligned} \frac{1}{2\delta_{1}}(\|u_{e}^{0}\|_{2}^{2} - \|u_{e}^{K+1}\|_{2}^{2}) &+ \frac{1}{2\delta_{2}}(\|v_{e}^{0}\|_{2}^{2} - \|v_{e}^{K+1}\|_{2}^{2}) + \frac{1}{2\delta_{3}}(\|w_{e}^{0}\|_{2}^{2} - \|w_{e}^{K+1}\|_{2}^{2}) \\ &+ \frac{\mu_{1}}{2}(\|a_{e}^{0}\|_{2}^{2} - \|a_{e}^{K+1}\|_{2}^{2}) + \frac{\mu_{2}}{2}(\|b_{e}^{0}\|_{2}^{2} - \|b_{e}^{K+1}\|_{2}^{2}) + \frac{\mu_{3}}{2}(\|c_{e}^{0}\|_{2}^{2} - \|c_{e}^{K+1}\|_{2}^{2}) \\ &= \lambda_{1}\sum_{k=0}^{K}\langle p^{k+1} - p^{*}, a^{k+1} - a^{*}\rangle + \lambda_{2}\sum_{k=0}^{K}\langle q^{k+1} - q^{*}, b^{k+1} - b^{*}\rangle \\ &+ \frac{1}{n}\sum_{k=0}^{K}\langle s^{k+1} - s^{*}, c^{k+1} - c^{*}\rangle + \frac{\mu_{1}}{2}\sum_{k=0}^{K}\|\beta_{e}^{k+1} - a_{e}^{k}\|_{2}^{2} + \frac{\mu_{1} - \delta_{1}}{2}\sum_{k=0}^{K}\|\beta_{e}^{k+1} - a_{e}^{k+1}\|_{2}^{2} \\ &+ \frac{\mu_{2}}{2}\sum_{k=0}^{K}\|L\beta_{e}^{k+1} - b_{e}^{k}\|_{2}^{2} + \frac{\mu_{2} - \delta_{2}}{2}\sum_{k=0}^{K}\|L\beta_{e}^{k+1} - b_{e}^{k+1}\|_{2}^{2} \\ &+ \frac{\mu_{3}}{2}\sum_{k=0}^{K}\|YX\beta_{e}^{k+1} + y\beta_{0e}^{k+1} + c_{e}^{k}\|_{2}^{2} + \frac{\mu_{3} - \delta_{3}}{2}\sum_{k=0}^{K}\|YX\beta_{e}^{k+1} + \beta_{0e}^{k+1}\|y + c_{e}^{k+1}\|_{2}^{2}. \end{aligned}$$

$$(58)$$

The fact $p^{k+1} \in \partial ||a^{k+1}||_1, p^* \in \partial ||a^*||$ and $|| \cdot ||_1$ is convex implies $\langle p^{k+1} - p^*, a^{k+1} - a^* \rangle \geq 0$. Similarly, $\langle q^{k+1} - q^*, b^{k+1} - b^* \rangle \geq 0, \langle s^{k+1} - s^*, c^{k+1} - c^* \rangle \geq 0$. Therefore, all terms involved in (58) are nonnegative. Now we can cheat each term in the right hand side of (58) separately by the same argument as the proof of Theorem 1 and get the convergence result (21). The proof of (22) can also follows the same line as the one of Theorem 1, we omit the details here.

A.3. Updates in SBFLSVM

A.3.1. Update of β

Due to the extra bias term of β_0^{k+1} , we need to solve the following linear system which is slightly different from (14).

$$\begin{pmatrix} \mu_{1}I + \mu_{2}L^{T}L + \mu_{3}X^{T}Y^{2}X & \mu_{3}X^{T}Yy \\ \mu_{3}y^{T}YX & \mu_{3}y^{T}y \end{pmatrix} \begin{pmatrix} \beta^{k+1} \\ \beta_{0}^{k+1} \end{pmatrix}$$

$$= \mu_{1} \begin{pmatrix} a^{k} - \mu_{1}^{-1}u^{k} \\ 0 \end{pmatrix} + \mu_{2} \begin{pmatrix} L^{T} \\ 0 \end{pmatrix} (b^{k} - \mu_{2}^{-1}v^{k}) + \mu_{3} \begin{pmatrix} X^{T}Y \\ y^{T} \end{pmatrix} (\mathbf{1} - c^{k} + \mu_{3}^{-1}w^{k})$$

$$(59)$$

Fortunately, this linear system can also be solved by PCG efficiently. Note that

$$\begin{pmatrix} \mu_1 I + \mu_2 L^T L + \mu_3 X^T Y^2 X & \mu_3 X^T Y y \\ \mu_3 y^T Y X & \mu_3 y^T y \end{pmatrix}$$

= $\begin{pmatrix} \mu_1 I + \mu_2 L^T L & 0 \\ 0 & \mu_3 y^T y \end{pmatrix} + \mu_3 \begin{pmatrix} X^T Y \\ y^T \end{pmatrix} (YX, y) - \begin{pmatrix} 0 & 0 \\ 0 & \mu_3 y^T y \end{pmatrix} .$

It is easy to see that $\begin{pmatrix} \mu_1 I + \mu_2 L^T L & 0\\ 0 & \mu_3 y^T y \end{pmatrix}$ is still a tridiagonal matrix and

$$\mu_3 \begin{pmatrix} X^T Y \\ y^T \end{pmatrix} (YX,y) - \begin{pmatrix} 0 & 0 \\ 0 & \mu_3 y^T y \end{pmatrix}$$

is a low rank matrix. So PCG is still a good solver for the linear system (59).

A.3.2. Proof of Proposition 1

Proof. The energy function $\lambda x_+ + \frac{1}{2} ||x - w||_2^2$ is strongly convex, hence has a unique minimizer. Therefore, by the subdifferential calculus (c.f. [28]), s_{λ} is the unique solution of the following equation with unknown w

$$0 \in \lambda \partial(x_+) + x - w, \tag{60}$$

where $\partial(x_+) = \{p \in \mathbb{R} : y_+ - x_+ - (y - x)p \ge 0, \forall y \in \mathbb{R}\}$ is the subdifferential of the function x_+ . If $x \ne 0$, then x_+ is differentiable, and its subdifferential contains only its gradient. If x = 0, then $\partial(x_+) = \{p \in \mathbb{R} : y_+ - yp \ge 0, \forall y \in \mathbb{R}\}$. One can check that $\partial(x_+) = \{p : 0 \le p \le 1\}$ for this case. Indeed, for any $p \in [0, 1]$, $yp \le y_+$ by using the definition of y_+ . On the other hand, if there exists a number $p \in (-\infty, 0) \cup (1, +\infty)$ and $p \in \partial(x_+)$, then we can easily get a contraction. Actually, the fact $p \in (-\infty, 0) \cup (1, +\infty)$ implies $p^2 > p_+$. On the other hand, since $\partial(x_+) = \{p \in \mathbb{R} : y_+ - yp \ge 0, \forall y \in \mathbb{R}\}$ for x = 0, we have $p^2 < p_+$ by letting y = p. In summary,

$$\partial(x_{+}) = \begin{cases} 1, & x > 0, \\ \{p : p \in [0, 1]\}, & x = 0, \\ 0, & x < 0. \end{cases}$$
(61)

With (60) and (61), we can get the desired result.