A General Iterative Shrinkage and Thresholding Algorithm for Non-convex Regularized Optimization Problems

Pinghua Gong   GPH08@MAILS.TSINGHUA.EDU.CN
Changshui Zhang   ZCS@MAIL.TSINGHUA.EDU.CN
State Key Laboratory on Intelligent Technology and Systems
Tsinghua National Laboratory for Information Science and Technology (TNList)
Department of Automation, Tsinghua University, Beijing 100084, China

Zhaosong Lu   ZHAOSONG@SFU.CA
Department of Mathematics, Simon Fraser University, Burnaby, BC, V5A 1S6, Canada

Jianhua Z. Huang   JIANHUA@STAT.TAMU.EDU
Department of Statistics, Texas A&M University, TX 77843, USA

Jieping Ye   JIEPING.YE@ASU.EDU
Computer Science and Engineering, Arizona State University, Tempe, AZ 85287, USA

Abstract

Non-convex sparsity-inducing penalties have recently received considerable attentions in sparse learning. Recent theoretical investigations have demonstrated their superiority over the convex counterparts in several sparse learning settings. However, solving the non-convex optimization problems associated with non-convex penalties remains a big challenge. A commonly used approach is the Multi-Stage (MS) convex relaxation (or DC programming), which relaxes the original non-convex problem to a sequence of convex problems. This approach is usually not very practical for large-scale problems because its computational cost is a multiple of solving a single convex problem. In this paper, we propose a General Iterative Shrinkage and Thresholding (GIST) algorithm to solve the nonconvex optimization problem for a large class of non-convex penalties. The GIST algorithm iteratively solves a proximal operator problem, which in turn has a closed-form solution for many commonly used penalties. At each outer iteration of the algorithm, we use a line search initialized by the Barzilai-Borwein (BB) rule that allows finding an appropriate step size quickly. The paper also presents a detailed convergence analysis of the GIST algorithm. The efficiency of the proposed algorithm is demonstrated by extensive experiments on large-scale data sets.

1. Introduction

Learning sparse representations has important applications in many areas of science and engineering. The use of an ℓ_0-norm regularizer leads to a sparse solution, however the ℓ_0-norm regularized optimization problem is challenging to solve, due to the discontinuity and non-convexity of the ℓ_0-norm regularizer. The ℓ_1-norm regularizer, a continuous and convex surrogate, has been studied extensively in the literature (Tibshirani, 1996; Efron et al., 2004) and has been applied successfully to many applications including signal/image processing, biomedical informatics and computer vision (Shevade & Keerthi, 2003; Wright et al., 2008; Beck & Teboulle, 2009; Wright et al., 2009; Ye & Liu, 2012). Although the ℓ_1-norm based sparse learning formulations have achieved great success, they have been shown to be suboptimal in many cases (Candes et al., 2008; Zhang, 2010b; 2012), since the ℓ_1-norm is a loose approximation of the ℓ_0-norm and often leads to an over-penalized problem. To address this issue, many non-convex regularizers, interpolated between the ℓ_0-norm and

the ℓ_1-norm, have been proposed to better approximate the ℓ_0-norm. They include ℓ_q-norm ($0 < q < 1$) (Foucart & Lai, 2009), Smoothly Clipped Absolute Deviation (SCAD) (Fan & Li, 2001), Log-Sum Penalty (LSP) (Candes et al., 2008), Minimax Concave Penalty (MCP) (Zhang, 2010a), Geman Penalty (GP) (Geman & Yang, 1995; Trzasko & Manduca, 2009) and Capped-ℓ_1 penalty (Zhang, 2010b; 2012; Gong et al., 2012a).

Although the non-convex regularizers (penalties) are appealing in sparse learning, it is challenging to solve the corresponding non-convex optimization problems. In this paper, we propose a General Iterative Shrinkage and Thresholding (GIST) algorithm for a large class of non-convex penalties. The key step of the proposed algorithm is to compute a proximal operator, which has a closed-form solution for many commonly used non-convex penalties. In our algorithm, we adopt the Barzilai-Borwein (BB) rule (Barzilai & Borwein, 1988) to initialize the line search step size at each iteration, which greatly accelerates the convergence speed. We also use a non-monotone line search criterion to further speed up the convergence of the algorithm. In addition, we present a detailed convergence analysis for the proposed algorithm. Extensive experiments on large-scale real-world data sets demonstrate the efficiency of the proposed algorithm.

2. The Proposed Algorithm: GIST

2.1. General Problems

We consider solving the following general problem:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \left\{ f(\mathbf{w}) = l(\mathbf{w}) + r(\mathbf{w}) \right\}. \tag{1}$$

We make the following assumptions on the above formulation throughout the paper:

A1 $l(\mathbf{w})$ is continuously differentiable with Lipschitz continuous gradient, that is, there exists a positive constant $\beta(l)$ such that

$$\|\nabla l(\mathbf{w}) - \nabla l(\mathbf{u})\| \le \beta(l)\|\mathbf{w} - \mathbf{u}\|, \forall \mathbf{w}, \mathbf{u} \in \mathbb{R}^d.$$

A2 $r(\mathbf{w})$ is a continuous function which is possibly *non-smooth* and *non-convex*, and can be rewritten as the difference of two convex functions, that is,

$$r(\mathbf{w}) = r_1(\mathbf{w}) - r_2(\mathbf{w}),$$

where $r_1(\mathbf{w})$ and $r_2(\mathbf{w})$ are convex functions.

A3 $f(\mathbf{w})$ is bounded from below.

Remark 1 *We say that $\mathbf{w}^\star$ is a critical point of problem (1), if the following holds (Toland, 1979; Wright et al., 2009):*

$$\mathbf{0} \in \nabla l(\mathbf{w}^\star) + \partial r_1(\mathbf{w}^\star) - \partial r_2(\mathbf{w}^\star),$$

where $\partial r_1(\mathbf{w}^\star)$ is the sub-differential of the function $r_1(\mathbf{w})$ at $\mathbf{w} = \mathbf{w}^\star$, that is,

$$\partial r_1(\mathbf{w}^\star) = \left\{ \mathbf{s} : r_1(\mathbf{w}) \ge r_1(\mathbf{w}^\star) + \langle \mathbf{s}, \mathbf{w} - \mathbf{w}^\star \rangle, \forall \mathbf{w} \in \mathbb{R}^d \right\}.$$

We should mention that the sub-differential is non-empty on any convex function; this is why we make the assumption that $r(\mathbf{w})$ can be rewritten as the difference of two convex functions.

2.2. Some Examples

Many formulations in machine learning satisfy the assumptions above. The following least square and logistic loss functions are two commonly used ones which satisfy assumption **A1**:

$$l(\mathbf{w}) = \frac{1}{2n}\|X\mathbf{w} - \mathbf{y}\|^2 \text{ or } \frac{1}{n}\sum_{i=1}^{n} \log\left(1 + \exp(-y_i\mathbf{x}_i^T\mathbf{w})\right),$$

where $X = [\mathbf{x}_1^T; \cdots; \mathbf{x}_n^T] \in \mathbb{R}^{n \times d}$ is a data matrix and $\mathbf{y} = [y_1, \cdots, y_n]^T \in \mathbb{R}^n$ is a target vector. The regularizers (penalties) which satisfy the assumption **A2** are presented in Table 1. They are non-convex (except the ℓ_1-norm) and extensively used in sparse learning. The functions $l(\mathbf{w})$ and $r(\mathbf{w})$ mentioned above are nonnegative. Hence, f is bounded from below and satisfies assumption **A3**.

2.3. Algorithm

Our proposed General Iterative Shrinkage and Thresholding (GIST) algorithm solves problem (1) by generating a sequence $\{\mathbf{w}^{(k)}\}$ via:

$$\mathbf{w}^{(k+1)} = \arg\min_{\mathbf{w}} \ l(\mathbf{w}^{(k)}) + \langle \nabla l(\mathbf{w}^{(k)}), \mathbf{w} - \mathbf{w}^{(k)} \rangle$$
$$+ \frac{t^{(k)}}{2}\|\mathbf{w} - \mathbf{w}^{(k)}\|^2 + r(\mathbf{w}), \tag{2}$$

In fact, problem (2) is equivalent to the following proximal operator problem:

$$\mathbf{w}^{(k+1)} = \arg\min_{\mathbf{w}} \ \frac{1}{2}\|\mathbf{w} - \mathbf{u}^{(k)}\|^2 + \frac{1}{t^{(k)}}r(\mathbf{w}),$$

where $\mathbf{u}^{(k)} = \mathbf{w}^{(k)} - \nabla l(\mathbf{w}^{(k)})/t^{(k)}$. Thus, in GIST we first perform a gradient descent along the direction $-\nabla l(\mathbf{w}^{(k)})$ with step size $1/t^{(k)}$ and then solve a proximal operator problem. For all the regularizers listed in Table 1, problem (2) has a closed-form solution (details are provided in the Appendix), although it may

Table 1. Examples of regularizers (penalties) $r(\mathbf{w})$ satisfying the assumption **A2** and the corresponding convex functions $r_1(\mathbf{w})$ and $r_2(\mathbf{w})$. $\lambda > 0$ is the regularization parameter; $r(\mathbf{w}) = \sum_i r_i(w_i), r_1(\mathbf{w}) = \sum_i r_{1,i}(w_i), r_2(\mathbf{w}) = \sum_i r_{2,i}(w_i), [x]_+ = \max(0, x)$.

Name	$r_i(w_i)$	$r_{1,i}(w_i)$	$r_{2,i}(w_i)$
ℓ_1-norm	$\lambda|w_i|$	$\lambda|w_i|$	0
LSP	$\lambda \log(1 + |w_i|/\theta) \ (\theta > 0)$	$\lambda|w_i|$	$\lambda(|w_i| - \log(1 + |w_i|/\theta))$
SCAD	$\lambda \int_0^{|w_i|} \min\left(1, \frac{[\theta\lambda - x]_+}{(\theta-1)\lambda}\right) dx \ (\theta > 2)$ $= \begin{cases} \lambda|w_i|, & \text{if } |w_i| \leq \lambda, \\ \frac{-w_i^2 + 2\theta\lambda|w_i| - \lambda^2}{2(\theta-1)}, & \text{if } \lambda < |w_i| \leq \theta\lambda, \\ (\theta+1)\lambda^2/2, & \text{if } |w_i| > \theta\lambda. \end{cases}$	$\lambda|w_i|$	$\lambda \int_0^{|w_i|} \frac{[\min(\theta\lambda, x) - \lambda]_+}{(\theta-1)\lambda} dx$ $= \begin{cases} 0, & \text{if } |w_i| \leq \lambda, \\ \frac{w_i^2 - 2\lambda|w_i| + \lambda^2}{2(\theta-1)}, & \text{if } \lambda < |w_i| \leq \theta\lambda, \\ \lambda|w_i| - \frac{(\theta+1)\lambda^2}{2}, & \text{if } |w_i| > \theta\lambda. \end{cases}$
MCP	$\lambda \int_0^{|w_i|} \left[1 - \frac{x}{\theta\lambda}\right]_+ dx \ (\theta > 0)$ $= \begin{cases} \lambda|w_i| - w_i^2/(2\theta), & \text{if } |w_i| \leq \theta\lambda, \\ \theta\lambda^2/2, & \text{if } |w_i| > \theta\lambda. \end{cases}$	$\lambda|w_i|$	$\lambda \int_0^{|w_i|} \min(1, x/(\theta\lambda)) dx$ $= \begin{cases} w_i^2/(2\theta), & \text{if } |w_i| \leq \theta\lambda, \\ \lambda|w_i| - \theta\lambda^2/2, & \text{if } |w_i| > \theta\lambda. \end{cases}$
Capped ℓ_1	$\lambda \min(|w_i|, \theta) \ (\theta > 0)$	$\lambda|w_i|$	$\lambda[|w_i| - \theta]_+$

Algorithm 1 GIST: General Iterative Shrinkage and Thresholding Algorithm

1: Choose parameters $\eta > 1$ and $t_{\min}, t_{\max}$ with $0 < t_{\min} < t_{\max}$;
2: Initialize iteration counter $k \leftarrow 0$ and a bounded starting point $\mathbf{w}^{(0)}$;
3: **repeat**
4:    $t^{(k)} \in [t_{\min}, t_{\max}]$;
5:    **repeat**
6:       $\mathbf{w}^{(k+1)} \leftarrow \arg\min_{\mathbf{w}} \ l(\mathbf{w}^{(k)}) + \langle \nabla l(\mathbf{w}^{(k)}), \mathbf{w} - \mathbf{w}^{(k)} \rangle + \frac{t^{(k)}}{2}\|\mathbf{w} - \mathbf{w}^{(k)}\|^2 + r(\mathbf{w})$;
7:       $t^{(k)} \leftarrow \eta t^{(k)}$;
8:    **until** some line search criterion is satisfied
9:    $k \leftarrow k + 1$
10: **until** some stopping criterion is satisfied

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be a non-convex problem. For example, for the ℓ_1 and Capped ℓ_1 regularizers, we have closed-form solutions as follows:

$$\ell_1 : w_i^{(k+1)} = \text{sign}(u_i^{(k)}) \max\left(0, |u_i^{(k)}| - \lambda/t^{(k)}\right),$$

$$\text{Capped } \ell_1 : w_i^{(k+1)} = \begin{cases} x_1, & \text{if } h_i(x_1) \leq h_i(x_2), \\ x_2, & \text{otherwise,} \end{cases}$$

where $x_1 = \text{sign}(u_i^{(k)}) \max(|u_i^{(k)}|, \theta)$, $x_2 = \text{sign}(u_i^{(k)}) \min(\theta, [|u_i^{(k)}| - \lambda/t^{(k)}]_+)$ and $h_i(x) = 0.5(x - u_i^{(k)})^2 + \lambda/t^{(k)} \min(|x|, \theta)$. The detailed procedure of the GIST algorithm is presented in Algorithm 1. There are two issues that remain to be addressed: how to initialize $t^{(k)}$ (in Line 4) and how to select a line search criterion (in Line 8) at each outer iteration.

2.3.1. THE STEP SIZE INITIALIZATION: $1/t^{(k)}$

Intuitively, a good step size initialization strategy at each outer iteration can greatly reduce the line search cost (Lines 5-8) and hence is critical for the fast con-

vergence of the algorithm. In this paper, we propose to initialize the step size by adopting the Barzilai-Borwein (BB) rule (Barzilai & Borwein, 1988), which uses a diagonal matrix $t^{(k)}I$ to approximate the Hessian matrix $\nabla^2 l(\mathbf{w})$ at $\mathbf{w} = \mathbf{w}^{(k)}$. Denote

$$\mathbf{x}^{(k)} = \mathbf{w}^{(k)} - \mathbf{w}^{(k-1)}, \ \mathbf{y}^{(k)} = \nabla l(\mathbf{w}^{(k)}) - \nabla l(\mathbf{w}^{(k-1)}).$$

Then $t^{(k)}$ is initialized at the outer iteration k as

$$t^{(k)} = \arg\min_t \|t\mathbf{x}^{(k)} - \mathbf{y}^{(k)}\|^2 = \frac{\langle \mathbf{x}^{(k)}, \mathbf{y}^{(k)} \rangle}{\langle \mathbf{x}^{(k)}, \mathbf{x}^{(k)} \rangle}.$$

2.3.2. LINE SEARCH CRITERION

One natural and commonly used line search criterion is to require that the objective function value is monotonically decreasing. More specifically, we propose to accept the step size $1/t^{(k)}$ at the outer iteration k if the following monotone line search criterion is satisfied:

$$f(\mathbf{w}^{(k+1)}) \leq f(\mathbf{w}^{(k)}) - \frac{\sigma}{2}t^{(k)}\|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2, \quad (3)$$

where σ is a constant in the interval $(0, 1)$.

A variant of the monotone criterion in Eq. (3) is a non-monotone line search criterion (Grippo et al., 1986; Grippo & Sciandrone, 2002; Wright et al., 2009). It possibly accepts the step size $1/t^{(k)}$ even if $\mathbf{w}^{(k+1)}$ yields a larger objective function value than $\mathbf{w}^{(k)}$. Specifically, we propose to accept the step size $1/t^{(k)}$, if $\mathbf{w}^{(k+1)}$ makes the objective function value smaller than the maximum over previous $m \ (m > 1)$ iterations, that is,

$$f(\mathbf{w}^{(k+1)}) \leq \max_{i=\max(0,k-m+1),\cdots,k} f(\mathbf{w}^{(i)}) - \frac{\sigma}{2}t^{(k)}\|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2, \quad (4)$$

where $\sigma \in (0, 1)$.

2.3.3. CONVERGENCE ANALYSIS

Inspired by Wright et al. (2009); Lu (2012a), we present detailed convergence analysis under both monotone and non-monotone line search criteria. We first present a lemma which guarantees that the monotone line search criterion in Eq. (3) is satisfied. This is a basic support for the convergence of Algorithm 1.

Lemma 1 *Let the assumptions $\mathbf{A1}$-$\mathbf{A3}$ hold and the constant $\sigma \in (0,1)$ be given. Then for any integer $k \geq 0$, the monotone line search criterion in Eq. (3) is satisfied whenever $t^{(k)} \geq \beta(l)/(1-\sigma)$.*

Proof Since $\mathbf{w}^{(k+1)}$ is a minimizer of problem (2), we have

$$\langle \nabla l(\mathbf{w}^{(k)}), \mathbf{w}^{(k+1)} - \mathbf{w}^{(k)} \rangle + \frac{t^{(k)}}{2} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2$$
$$+ r(\mathbf{w}^{(k+1)}) \leq r(\mathbf{w}^{(k)}). \tag{5}$$

It follows from assumption **A1** that

$$l(\mathbf{w}^{(k+1)}) \leq l(\mathbf{w}^{(k)}) + \langle \nabla l(\mathbf{w}^{(k)}), \mathbf{w}^{(k+1)} - \mathbf{w}^{(k)} \rangle$$
$$+ \frac{\beta(l)}{2} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2. \tag{6}$$

Combining Eq. (5) and Eq. (6), we have

$$l(\mathbf{w}^{(k+1)}) + r(\mathbf{w}^{(k+1)}) \leq l(\mathbf{w}^{(k)}) + r(\mathbf{w}^{(k)})$$
$$- \frac{t^{(k)} - \beta(l)}{2} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2.$$

It follows that

$$f(\mathbf{w}^{(k+1)}) \leq f(\mathbf{w}^{(k)}) - \frac{t^{(k)} - \beta(l)}{2} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2.$$

Therefore, the line search criterion in Eq. (3) is satisfied whenever $(t^{(k)} - \beta(l))/2 \geq \sigma t^{(k)}/2$, i.e., $t^{(k)} \geq \beta(l)/(1-\sigma)$. This completes the proof the lemma. $\square$

Next, we summarize the boundedness of $t^{(k)}$ in the following lemma.

Lemma 2 *For any $k \geq 0$, $t^{(k)}$ is bounded under the monotone line search criterion in Eq. (3).*

Proof It is trivial to show that $t^{(k)}$ is bounded from below, since $t^{(k)} \geq t_{\min}$ ($t_{\min}$ is defined in Algorithm 1). Next we prove that $t^{(k)}$ is bounded from above by contradiction. Assume that there exists a $k \geq 0$, such that $t^{(k)}$ is unbounded from above. Without loss of generality, we assume that $t^{(k)}$ increases monotonically to $+\infty$ and $t^{(k)} \geq \eta\beta(l)/(1-\sigma)$. Thus, the value $t = t^{(k)}/\eta \geq \beta(l)/(1-\sigma)$ must have been tried at iteration k and does not satisfy the line search criterion in Eq. (3). But Lemma 1 states that $t = t^{(k)}/\eta \geq \beta(l)/(1-\sigma)$ is guaranteed to satisfy the line search criterion in Eq. (3). This leads to a contradiction. Thus, $t^{(k)}$ is bounded from above. $\square$

Remark 2 *We note that if Eq. (3) holds, Eq. (4) is guaranteed to be satisfied. Thus, the same conclusions in Lemma 1 and Lemma 2 also hold under the the non-monotone line search criterion in Eq. (4).*

Based on Lemma 1 and Lemma 2, we present our convergence result in the following theorem.

Theorem 1 *Let the assumptions $\mathbf{A1}$-$\mathbf{A3}$ hold and the monotone line search criterion in Eq. (3) be satisfied. Then all limit points of the sequence $\{\mathbf{w}^{(k)}\}$ generated by Algorithm 1 are critical points of problem (1).*

Proof Based on Lemma 1, the monotone line search criterion in Eq. (3) is satisfied and hence

$$f(\mathbf{w}^{(k+1)}) \leq f(\mathbf{w}^{(k)}), \forall k \geq 0,$$

which implies that the sequence $\{f(\mathbf{w}^{(k)})\}_{k=0,1,\cdots}$ is monotonically decreasing. Let $\mathbf{w}^\star$ be a limit point of the sequence $\{\mathbf{w}^{(k)}\}$, that is, there exists a subsequence $\mathcal{K}$ such that

$$\lim_{k \in \mathcal{K} \to \infty} \mathbf{w}^{(k)} = \mathbf{w}^\star.$$

Since f is bounded from below, together with the fact that $\{f(\mathbf{w}^{(k)})\}$ is monotonically decreasing, $\lim_{k\to\infty} f(\mathbf{w}^{(k)})$ exists. Observing that f is continuous, we have

$$\lim_{k \to \infty} f(\mathbf{w}^{(k)}) = \lim_{k \in \mathcal{K} \to \infty} f(\mathbf{w}^{(k)}) = f(\mathbf{w}^\star).$$

Taking limits on both sides of Eq. (3) with $k \in \mathcal{K}$, we have

$$\lim_{k \in \mathcal{K} \to \infty} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\| = 0. \tag{7}$$

Considering that the minimizer $\mathbf{w}^{(k+1)}$ is also a critical point of problem (2) and $r(\mathbf{w}) = r_1(\mathbf{w}) - r_2(\mathbf{w})$, we have

$$\mathbf{0} \in \nabla l(\mathbf{w}^{(k)}) + t^{(k)}(\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)})$$
$$+ \partial r_1(\mathbf{w}^{(k+1)}) - \partial r_2(\mathbf{w}^{(k+1)}).$$

Taking limits on both sides of the above equation with $k \in \mathcal{K}$, by considering the semi-continuity of $\partial r_1(\cdot)$ and $\partial r_2(\cdot)$, the boundedness of $t^{(k)}$ (based on Lemma 2) and Eq. (7), we obtain

$$\mathbf{0} \in \nabla l(\mathbf{w}^\star) + \partial r_1(\mathbf{w}^\star) - \partial r_2(\mathbf{w}^\star),$$

Therefore, $\mathbf{w}^\star$ is a critical point of problem (1). This completes the proof of Theorem 1. $\square$

Based on Eq. (7), we know that $\lim_{k \in \mathcal{K} \to \infty} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2 = 0$ is a necessary optimality condition of Algorithm 1. Thus, $\|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2$ is a quantity to measure the convergence of the sequence $\{\mathbf{w}^{(k)}\}$ to a critical point. We present the convergence rate in terms of $\|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2$ in the following theorem.

Theorem 2 *Let $\{\mathbf{w}^{(k)}\}$ be the sequence generated by Algorithm 1 with the monotone line search criterion in Eq. (3) satisfied. Then for every $n \geq 1$, we have*

$$\min_{0 \leq k \leq n} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2 \leq \frac{2(f(\mathbf{w}^{(0)}) - f(\mathbf{w}^\star))}{n \sigma t_{\min}},$$

where $\mathbf{w}^\star$ is a limit point of the sequence $\{\mathbf{w}^{(k)}\}$.

Proof Based on Eq. (3) with $t^{(k)} \geq t_{\min}$, we have

$$\frac{\sigma t_{\min}}{2} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2 \leq f(\mathbf{w}^{(k)}) - f(\mathbf{w}^{(k+1)}).$$

Summing the above inequality over $k = 0, \cdots, n$, we obtain

$$\frac{\sigma t_{\min}}{2} \sum_{k=0}^{n} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2 \leq f(\mathbf{w}^{(0)}) - f(\mathbf{w}^{(n+1)}),$$

which implies that

$$\min_{0 \leq k \leq n} \|\mathbf{w}^{(k+1)} - \mathbf{w}^{(k)}\|^2 \leq \frac{2(f(\mathbf{w}^{(0)}) - f(\mathbf{w}^{(n+1)}))}{n \sigma t_{\min}}$$
$$\leq \frac{2(f(\mathbf{w}^{(0)}) - f(\mathbf{w}^\star))}{n \sigma t_{\min}}.$$

This completes the proof of the theorem. □

Under the non-monotone line search criterion in Eq. (4), we have a similar convergence result in the following theorem (the proof uses an extension of argument for Theorem 1 and is omitted).

Theorem 3 *Let the assumptions **A1-A3** hold and the non-monotone line search criterion in Eq. (4) be satisfied. Then all limit points of the sequence $\{\mathbf{w}^{(k)}\}$ generated by Algorithm 1 are critical points of problem (1).*

Note that Theorem 1/Theorem 3 makes sense only if $\{\mathbf{w}^{(k)}\}$ has limit points. By considering one more mild assumption:

A4 $f(\mathbf{w}) \to +\infty$ when $\|\mathbf{w}\| \to +\infty$,

we summarize the existence of limit points in the following theorem (the proof is omitted):

Theorem 4 *Let the assumptions **A1-A4** hold and the monotone/non-monotone line search criterion in Eq. (3)/Eq. (4) be satisfied. Then the sequence $\{\mathbf{w}^{(k)}\}$ generated by Algorithm 1 has at least one limit point.*

2.3.4. DISCUSSIONS

Observe that $l(\mathbf{w}^{(k)}) + \langle \nabla l(\mathbf{w}^{(k)}), \mathbf{w} - \mathbf{w}^{(k)} \rangle + \frac{t^{(k)}}{2} \|\mathbf{w} - \mathbf{w}^{(k)}\|^2$ can be viewed as an approximation of $l(\mathbf{w})$ at $\mathbf{w} = \mathbf{w}^{(k)}$. The GIST algorithm minimizes an approximate surrogate instead of the objective function in problem (1) at each outer iteration. We further observe that if $t^{(k)} \geq \beta(l)/(1 - \sigma) > \beta(l)$ [the sufficient condition of Eq. (3)], we obtain

$$l(\mathbf{w}) \leq l(\mathbf{w}^{(k)}) + \langle \nabla l(\mathbf{w}^{(k)}), \mathbf{w} - \mathbf{w}^{(k)} \rangle$$
$$+ \frac{t^{(k)}}{2} \|\mathbf{w} - \mathbf{w}^{(k)}\|^2, \forall \mathbf{w} \in \mathbb{R}^d.$$

It follows that

$$f(\mathbf{w}) = l(\mathbf{w}) + r(\mathbf{w}) \leq M(\mathbf{w}, \mathbf{w}^{(k)}), \forall \mathbf{w} \in \mathbb{R}^d,$$

where $M(\mathbf{w}, \mathbf{w}^{(k)})$ denotes the objective function of problem (2). We can easily show that

$$f(\mathbf{w}^{(k)}) = M(\mathbf{w}^{(k)}, \mathbf{w}^{(k)}).$$

Thus, the GIST algorithm is equivalent to solving a sequence of minimization problems:

$$\mathbf{w}^{(k+1)} = \arg\min_{\mathbf{w}} M(\mathbf{w}, \mathbf{w}^{(k)}), \ k = 0, 1, 2, \cdots$$

and can be interpreted as the well-known Majorization and Minimization (MM) technique (Hunter & Lange, 2000).

Note that we focus on the vector case in this paper and the proposed GIST algorithm can be easily extended to the matrix case.

3. Related Work

In this section, we discuss some related algorithms. One commonly used approach to solve problem (1) is the Multi-Stage (MS) convex relaxation (or CCCP, or DC programming) (Zhang, 2010b; Yuille & Rangarajan, 2003; Gasso et al., 2009). It equivalently rewrites problem (1) as

$$\min_{\mathbf{w} \in \mathbb{R}^d} f_1(\mathbf{w}) - f_2(\mathbf{w}),$$

where $f_1(\mathbf{w})$ and $f_2(\mathbf{w})$ are both convex functions. The MS algorithm solves problem (1) by generating a sequence $\{\mathbf{w}^{(k)}\}$ as

$$\mathbf{w}^{(k+1)} = \arg\min_{\mathbf{w} \in \mathbb{R}^d} f_1(\mathbf{w}) - f_2(\mathbf{w}^{(k)})$$
$$- \langle \mathbf{s}_2(\mathbf{w}^{(k)}), \mathbf{w} - \mathbf{w}^{(k)} \rangle, \quad (8)$$

where $\mathbf{s}_2(\mathbf{w}^{(k)})$ denotes a sub-gradient of $f_2(\mathbf{w})$ at $\mathbf{w} = \mathbf{w}^{(k)}$. Obviously, the objective function in problem (8) is convex. The MS algorithm involves solving a

sequence of convex optimization problems as in problem (8). In general, there is no closed-form solution to problem (8) and the computational cost of the MS algorithm is k times that of solving problem (8), where k is the number of outer iterations. This is computationally expensive especially for large scale problems.

A class of related algorithms called iterative shrinkage and thresholding (IST), which are also known as different names such as fixed point iteration and forward-backward splitting (Daubechies et al., 2004; Combettes & Wajs, 2005; Hale et al., 2007; Beck & Teboulle, 2009; Wright et al., 2009; Liu et al., 2009), have been extensively applied to solve problem (1). The key step is by generating a sequence $\{\mathbf{w}^{(k)}\}$ via solving problem (2). However, they require that the regularizer $r(\mathbf{w})$ is *convex* and some of them even require that both $l(\mathbf{w})$ and $r(\mathbf{w})$ are convex. Our proposed GIST algorithm is a more general framework, which can deal with a wider range of problems including both convex and non-convex cases.

Another related algorithm called a Variant of Iterative Reweighted L_α (VIRL) is recently proposed to solve the following optimization problem (Lu, 2012a):

$$\min_{\mathbf{w}\in\mathbb{R}^d}\left\{f(\mathbf{w})=l(\mathbf{w})+\lambda\sum_{i=1}^{d}(|w_i|^\alpha+\epsilon_i)^{q/\alpha}\right\},$$

where $\alpha\geq 1, 0<q<1, \epsilon_i>0$. VIRL solves the above problem by generating a sequence $\{\mathbf{w}^{(k)}\}$ as

$$\mathbf{w}^{(k+1)}=\arg\min_{\mathbf{w}\in\mathbb{R}^d}l(\mathbf{w}^{(k)})+\langle\nabla l(\mathbf{w}^{(k)}),\mathbf{w}-\mathbf{w}^{(k)}\rangle$$

$$+\frac{t^{(k)}}{2}\|\mathbf{w}-\mathbf{w}^{(k)}\|^2+\frac{\lambda q}{\alpha}\sum_{i=1}^{d}(|w_i^k|^\alpha+\epsilon_i)^{q/\alpha-1}|w_i|^\alpha.$$

In VIRL, $t^{(k-1)}$ is chosen as the initialization of $t^{(k)}$. The line search step in VIRL finds the smallest integer ℓ with $t^{(k)}=t^{(k-1)}\eta^\ell$ ($\eta>1$) such that

$$f(\mathbf{w}^{(k+1)})\leq f(\mathbf{w}^{(k)})-\frac{\sigma}{2}\|\mathbf{w}^{(k+1)}-\mathbf{w}^{(k)}\|^2\ (\sigma>0).$$

The most related algorithm to our propose GIST is the Sequential Convex Programming (SCP) proposed by Lu (2012b). SCP solves problem (1) by generating a sequence $\{\mathbf{w}^{(k)}\}$ as

$$\mathbf{w}^{(k+1)}=\arg\min_{\mathbf{w}\in\mathbb{R}^d}l(\mathbf{w}^{(k)})+\langle\nabla l(\mathbf{w}^{(k)}),\mathbf{w}-\mathbf{w}^{(k)}\rangle$$

$$+\frac{t^{(k)}}{2}\|\mathbf{w}-\mathbf{w}^{(k)}\|^2+r_1(\mathbf{w})-r_2(\mathbf{w}^{(k)})-\langle\mathbf{s}_2,\mathbf{w}-\mathbf{w}^{(k)}\rangle,$$

where $\mathbf{s}_2$ is a sub-gradient of $r_2(\mathbf{w})$ at $\mathbf{w}=\mathbf{w}^{(k)}$. Our algorithm differs from SCP in that the original regularizer $r(\mathbf{w})=r_1(\mathbf{w})-r_2(\mathbf{w})$ is used in the proximal

operator in problem (2), while $r_1(\mathbf{w})$ minus a locally linear approximation for $r_2(\mathbf{w})$ is adopted in SCP. We will show in the experiments that our proposed GIST algorithm is more efficient than SCP.

4. Experiments

4.1. Experimental Setup

We evaluate our GIST algorithm by considering the Capped ℓ_1 regularized logistic regression problem, that is $l(\mathbf{w})=\frac{1}{n}\sum_{i=1}^{n}\log\left(1+\exp(-y_i\mathbf{x}_i^T\mathbf{w})\right)$ and $r(\mathbf{w})=\lambda\sum_{i=1}^{d}\min(|w_i|,\theta)$. We compare our GIST algorithm with the Multi-Stage (MS) algorithm and the SCP algorithm in different settings using twelve data sets summarized in Table 2. These data sets are high dimensional and sparse. Two of them (news20, real-sim)[1] have been preprocessed as two-class data sets (Lin et al., 2008). The other ten[2] are multi-class data sets. We transform the multi-class data sets into two-class by labeling the first half of all classes as positive class, and the remaining classes as the negative class.

All algorithms are implemented in Matlab and executed on an Intel(R) Core(TM)2 Quad CPU (Q6600 @2.4GHz) with 8GB memory. We set $\sigma=10^{-5}, m=5, \eta=2, 1/t_{\min}=t_{\max}=10^{30}$ and choose the starting points $\mathbf{w}^{(0)}$ of all algorithms as zero vectors. We terminate all algorithms if the relative change of the two consecutive objective function values is less than 10^{-5} or the number of iterations exceeds 1000. The Matlab codes of the GIST algorithm are available online (Gong et al., 2013).

4.2. Experimental Evaluation and Analysis

We report the objective function value vs. CPU time plots with different parameter settings in Figure 1. From these figures, we have the following observations: (1) Both GISTbb-Monotone and GISTbb-Nonmonotone decrease the objective function value rapidly and they always have the fastest convergence speed, which shows that adopting the BB rule to initialize $t^{(k)}$ indeed greatly accelerates the convergence speed. Moreover, both GISTbb-Monotone and GISTbb-Nonmonotone algorithms achieve the smallest objective function values. (2) GISTbb-Nonmonotone may give rise to an increasing objective function value but finally converges and has a faster overall convergence speed than GISTbb-Monotone in most cases, which indicates that the non-monotone line search criterion can further accelerate the con-

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[1]http://www.csie.ntu.edu.tw/cjlin/libsvmtools/datasets/
[2]http://www.shi-zhong.com/software/docdata.zip

vergence speed. (3) SCPbb-Nonmonotone is comparable to GISTbb-Nonmonotone in several cases, however, it converges much slower and achieves much larger objective function values than those of GISTbb-Nonmonotone in the remaining cases. This demonstrates the superiority of using the original regularizer $r(\mathbf{w}) = r_1(\mathbf{w}) - r_2(\mathbf{w})$ in the proximal operator in problem (2). (4) GIST-1 has a faster convergence speed than GIST-$t^{(k-1)}$ in most cases, which demonstrates that it is a bad strategy to use $t^{(k-1)}$ to initialize $t^{(k)}$. This is because $\{t^{(k)}\}$ increases monotonically in this way, making the step size $1/t^{(k)}$ monotonically decreasing when the algorithm proceeds.

5. Conclusions

We propose an efficient iterative shrinkage and thresholding algorithm to solve a general class of non-convex optimization problems encountered in sparse learning. A critical step of the proposed algorithm is the computation of a proximal operator, which has a closed-form solution for many commonly used formulations. We propose to initialize the step size at each iteration using the BB rule and employ both monotone and non-monotone criteria as line search conditions, which greatly accelerate the convergence speed. Moreover, we provide a detailed convergence analysis of the proposed algorithm, showing that the algorithm converges under both monotone and non-monotone line search criteria. Experiments results on large-scale data sets demonstrate the fast convergence of the proposed algorithm.

In our future work, we will focus on analyzing the theoretical performance (e.g., prediction error bound, parameter estimation error bound etc.) of the solution obtained by the GIST algorithm. In addition, we plan to apply the proposed algorithm to solve the multi-task feature learning problem (Gong et al., 2012a;b).

Acknowledgements

Appendix: Solutions to Problem (2)

Observe that $r(\mathbf{w}) = \sum_{i=1}^{d} r_i(w_i)$ and problem (2) can be equivalently decomposed into d independent univariate optimization problems:

$$w_i^{(k+1)} = \arg\min_{w_i} h_i(w_i) = \frac{1}{2}\left(w_i - u_i^{(k)}\right)^2 + \frac{1}{t^{(k)}} r_i(w_i),$$

where $i = 1, \cdots, d$ and $u_i^{(k)}$ is the i-th entry of $\mathbf{u}^{(k)} = \mathbf{w}^{(k)} - \nabla l(\mathbf{w}^{(k)})/t^{(k)}$. To simplify the notations, we unclutter the above equation by removing the subscripts and supscripts as follows:

$$w^{(k+1)} = \arg\min_{w} h_i(w) = \frac{1}{2}\left(w - u\right)^2 + \frac{1}{t} r_i(w). \quad (9)$$

- **ℓ_1-norm**: $w^{(k+1)} = \text{sign}(u)\max\left(0, |u| - \lambda/t\right)$.

- **LSP**: We can obtain an optimal solution of problem (9) via: $w^{(k+1)} = \text{sign}(u)x$, where x is an optimal solution of the following problem:

$$x = \arg\min_{w} \frac{1}{2}\left(w - |u|\right)^2 + \frac{\lambda}{t}\log(1 + w/\theta)$$
$$s.t.\ w \geq 0.$$

Noting that the objective function above is differentiable in the interval $[0, +\infty)$ and the minimum of the above problem is either a stationary point (the first derivative is zero) or an endpoint of the feasible region, we have

$$x = \arg\min_{w \in \mathcal{C}} \frac{1}{2}\left(w - |u|\right)^2 + \frac{\lambda}{t}\log(1 + w/\theta),$$

where $\mathcal{C}$ is a set composed of 3 elements or 1 element. If $t^2(|u| - \theta)^2 - 4t(\lambda - t|u|\theta) \geq 0$,

$$\mathcal{C} = \Big\{0,$$
$$\left[\frac{t(|u| - \theta) + \sqrt{t^2(|u| - \theta)^2 - 4t(\lambda - t|u|\theta)}}{2t}\right]_+$$
$$\left[\frac{t(|u| - \theta) - \sqrt{t^2(|u| - \theta)^2 - 4t(\lambda - t|u|\theta)}}{2t}\right]_+\Big\}.$$

Otherwise, $\mathcal{C} = \{0\}$.

- **SCAD**: We can recast problem (9) into the following three problems:

$$x_1 = \arg\min_{w} \frac{1}{2}\left(w - u\right)^2 + \frac{\lambda}{t}|w| \quad s.t.\ |w| \leq \lambda,$$

$$x_2 = \arg\min_{w} \frac{1}{2}\left(w - u\right)^2$$
$$+ \frac{-w^2 + 2\theta(\lambda/t)|w| - (\lambda/t)^2}{2(\theta - 1)} \quad s.t.\ \lambda \leq |w| \leq \theta\lambda,$$

$$x_3 = \arg\min_{w} \frac{1}{2}\left(w - u\right)^2 + \frac{(\theta + 1)\lambda^2}{2t^2} \quad s.t. |w| \geq \theta\lambda.$$

We can easily obtain that (x_2 is obtained using the similar idea as **LSP** by considering that $\theta > 2$):

$$x_1 = \text{sign}(u)\min(\lambda, \max(0, |u| - \lambda/t)),$$
$$x_2 = \text{sign}(u)\min(\theta\lambda, \max(\lambda, \frac{t|u|(\theta - 1) - \theta\lambda}{t(\theta - 2)})),$$
$$x_3 = \text{sign}(u)\max(\theta\lambda, |u|).$$

Table 2. Data sets statistics: n is the number of samples and d is the dimensionality of the data.

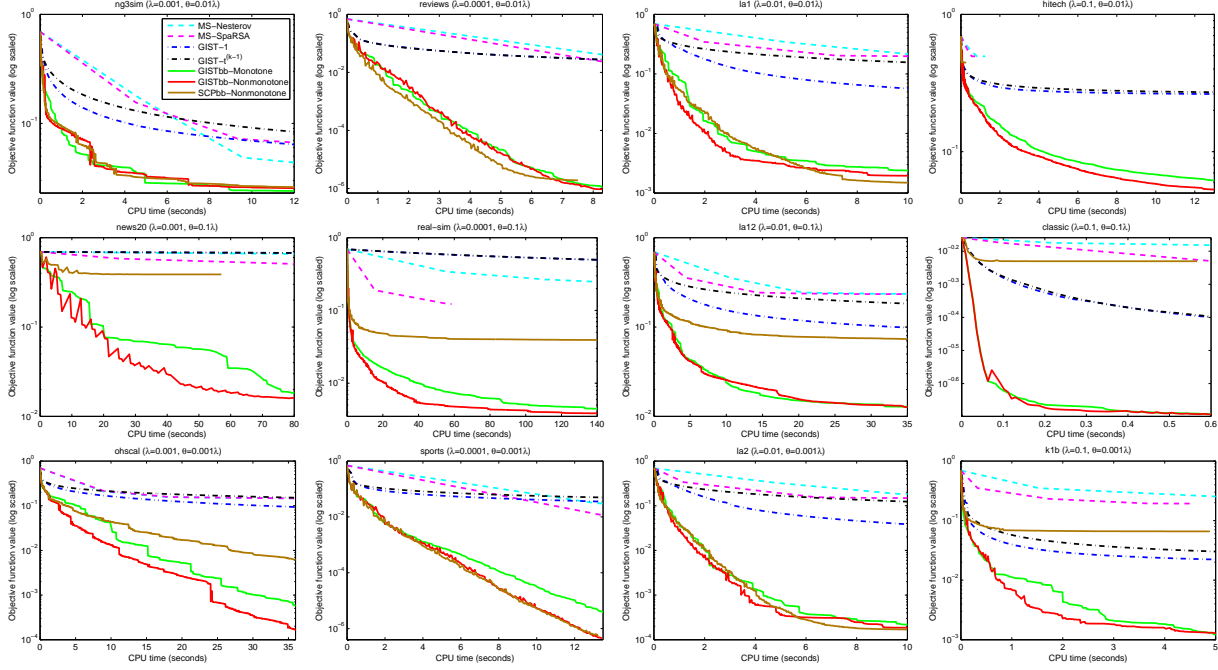| No.	1	2	3	4	5	6	7	8	9	10	11	12
datasets	classic	hitech	k1b	la12	la1	la2	news20	ng3sim	ohscal	real-sim	reviews	sports
n	7094	2301	2340	2301	3204	3075	19996	2998	11162	72309	4069	8580
d	41681	10080	21839	31472	31472	31472	1355191	15810	11465	20958	18482	14866

Figure 1. Objective function value vs. CPU time plots. MS-Nesterov/MS-SpaRSA: The Multi-Stage algorithm using the Nesterov/SpaRSA method to solve problem (8); GIST-1/GIST-$t^{(k-1)}$/GISTbb-Monotone/GISTbb-Nonmonotone: The GIST algorithm using $1/t^{(k-1)}$/BB rule/BB rule to initialize $t^{(k)}$ and Eq. (3)/Eq. (3)/Eq. (3)/Eq. (4) as the line search criterion; SCPbb-Nonmonotone: The SCP algorithm using the BB rule to initialize $t^{(k)}$ and Eq. (4) as the line search criterion. Note that on data sets 'hitech' and 'real-sim', MS algorithms stop early (the SCP algorithm has similar behaviors on data sets 'hitech' and 'news20'), because they satisfy the termination condition that the relative change of the two consecutive objective function values is less than 10^{-5}. However, their objective function values are much larger than those of GISTbb-Monotone and GISTbb-Nonmonotone.

Thus, we have

$$w^{(k+1)} = \underset{y}{\arg\min}\, h_i(y) \quad s.t.\ y \in \{x_1, x_2, x_3\}.$$

- **MCP**: Similar to SCAD, we can recast problem (9) into the following two problems:

$$x_1 = \underset{w}{\arg\min}\, \frac{1}{2}(w-u)^2 + \frac{\lambda}{t}|w| - \frac{w^2}{2\theta}\ s.t.\ |w| \le \theta\lambda,$$

$$x_2 = \underset{w}{\arg\min}\, \frac{1}{2}(w-u)^2 + \frac{\theta(\lambda/t)^2}{2}\ s.t.\ |w| \ge \theta\lambda.$$

We can easily obtain that

$$x_1 = \text{sign}(u)z,\ \ x_2 = \text{sign}(u)\max(\theta\lambda, |u|),$$

where $z = \arg\min_{w\in\mathcal{C}} \frac{1}{2}(w-|u|)^2 + \frac{\lambda}{t}w - \frac{w^2}{2\theta}$; $\mathcal{C} = \left\{0, \theta\lambda, \min\left(\theta\lambda, \max\left(0, \frac{\theta(t|u|-\lambda)}{t(\theta-1)}\right)\right)\right\}$, if $\theta - 1 \ne 0$,

and $\mathcal{C} = \{0, \theta\lambda\}$ otherwise. Thus, we have

$$w^{(k+1)} = \begin{cases} x_1, & \text{if } h_i(x_1) \le h_i(x_2) \\ x_2, & \text{otherwise.} \end{cases}$$

- **Capped ℓ_1**: We can recast problem (9) into the following two problems:

$$x_1 = \underset{w}{\arg\min}\, \frac{1}{2}(w-u)^2 + \frac{\lambda}{t}\theta \quad s.t.\ |w| \ge \theta,$$

$$x_2 = \underset{w}{\arg\min}\, \frac{1}{2}(w-u)^2 + \frac{\lambda}{t}|w| \quad s.t.\ |w| \le \theta.$$

We can easily obtain that

$$x_1 = \text{sign}(u)\max(\theta, |u|),$$
$$x_2 = \text{sign}(u)\min(\theta, \max(0, |u| - \lambda/t)).$$

Thus, we have

$$w^{(k+1)} = \begin{cases} x_1, & \text{if } h_i(x_1) \le h_i(x_2), \\ x_2, & \text{otherwise.} \end{cases}$$

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