Dynamic Sasvi: Strong Safe Screening for Norm-Regularized Least Squares

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Abstract

A recently introduced technique for a sparse optimization problem called "safe screening" allows us to identify irrelevant variables in the early stage of optimization. In this paper, we first propose a flexible framework for safe screening based on the Fenchel-Rockafellar duality and then derive a strong safe screening rule for norm-regularized least squares by the framework. We call the proposed screening rule for norm-regularized least squares "dynamic Sasvi" because it can be interpreted as a generalization of Sasvi. Unlike the original Sasvi, it does not require the exact solution of a more strongly regularized problem; hence, it works safely in practice. We show that our screening rule can eliminate more features and increase the speed of the solver in comparison with other screening rules both theoretically and experimentally.

1. Introduction

Sparse models such as Lasso (Tibshirani, 1996) and group Lasso (Yuan & Lin, 2006) have been widely studied in the areas of statistics and machine learning, and are used for various applications such as compressed sensing (Donoho, 2006) and biomarker discovery (Climente-González et al., 2019), to name a few. Although sparse models can be formulated as a simple convex optimization problem, the computational cost can be large if the numbers of samples and dimensions are extremely large.

To tackle this problem, a technique called safe screening has been introduced (Ghaoui et al., 2010) for Lasso problems. Specifically, it eliminates variables that are guaranteed to be zero in the Lasso solution before solving the original Lasso optimization problem. Many safe screening methods have been proposed for various problems (Ghaoui et al., 2010; Ogawa et al., 2013; Wang et al., 2015; Liu et al., 2014; Xiang et al., 2017). These are called sequential screening rules because they require the solution to a more strongly regularized problem. A recent technique used to eliminate variables through an estimated solution in an iterative solver, called dynamic screening, has been proposed (Bonnefoy et al., 2015). In particular, Gap Safe (Fercoq et al., 2015; Ndiaye et al., 2015), a dynamic screening framework is widely used owing to its generality and efficiency (Ndiaye et al., 2017; Shibagaki et al., 2016; Bao et al., 2020; Raj et al., 2016; Ndiaye et al., 2020). More specifically, Gap Safe efficiently screens variables by using the dual form of the original problems, where the screening is characterized by properly designing the dual safe region. For Lasso, two simple region-based approaches exist: Gap Safe Sphere and Gap Safe Dome (Fercoq et al., 2015).

In this paper, we propose a dynamic safe screening algorithm that is stronger than either Gap Safe Sphere or Gap Safe Dome for the Lasso-Like problem, which includes norm-regularized least squares. To this end, we first propose a general screening framework based on the Fenchel-Rockafellar duality and then derive Dynamic Sasvi, a strong safe screening rule for Lasso-like problems. Our framework can be regarded as a generalization of the Gap Safe framework, and thus we can derive Gap Safe Sphere and Gap Safe Dome simply using our results. Moreover, thanks to this generalization, we can use a strong problem adaptive inequality. Interestingly, the derived screening rule for Lasso-like problems can be seen as a dynamic variant of the safe screening with variational inequalities (Sasvi) (Liu et al., 2014), a sequential screening rule for Lasso. Therefore, we call this dynamic Sasvi. Unlike the original Sasvi, dynamic Sasvi does not require an exact solution to the problem with another hyper-parameter and hence operates safely in practice. Moreover, we propose the use of dynamic enhanced dual polytope projections (EDPP) (Wang et al., 2015), which are a relaxation of dynamic Sasvi by introducing a minimum radius sphere. We show both theoretically and experimentally that the screening power and computational costs of Dynamic Sasvi and Dynamic EDPP compare favorably with those of other state-of-the-art Gap Safe methods.

Contribution: The contributions of our paper are summarized as follows.

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• We propose a flexible screening framework based on Fenchel-Rockafellar duality, which is a generalization of the Gap Safe framework (Ndiaye et al., 2017).

• We propose two novel dynamic screening rules for norm-regularized least squares, which are a dynamic variant of Sasvi (Liu et al., 2014) and a dynamic variant of EDPP.

• We show that Dynamic Sasvi eliminates more features and increases the speed of the solver in comparison to Gap Safe (Fercoq et al., 2015; Ndiaye et al., 2017) both theoretically and experimentally.

2. Preliminary

In this section, we first formulate the problem and introduce the key techniques used in this study.

2.1. Notation

Given \( h : \mathbb{R}^m \to [-\infty, \infty] \), the domain of \( h \) is defined by

\[
\text{dom}(h) := \{ z \in \mathbb{R}^m \mid |h(z)| < \infty \}
\]

and \( h^* : \mathbb{R}^m \to [-\infty, \infty] \), the Fenchel conjugate of \( h \), is defined by

\[
h^*(v) := \sup_{z \in \mathbb{R}^d} v^\top z - h(z).
\]

If \( h \) is proper, the Fenchel-Young inequality

\[
h(z) + h^*(v) \geq v^\top z
\]

(1)
can be proven directly from the definition of the Fenchel conjugate. The subdifferential of a proper function \( h : \mathbb{R}^m \to (-\infty, \infty] \) at \( z \) is given as

\[
\partial h(z) := \{ v \in \mathbb{R}^m \mid \forall w \in \mathbb{R}^m : v^\top (w - z) + h(z) \leq h(w) \}.
\]

The next proposition is important for driving Safe-screening algorithms.

**Proposition 1** Assume that \( h : \mathbb{R}^m \to (-\infty, \infty] \) is a proper lower semicontinuous convex function and \( z, v \in \mathbb{R}^m \). We then have

\[
\begin{align*}
\forall v \in \partial h(z) & \iff h(z) + h^*(v) = v^\top z \\
& \iff z \in \partial h^*(v).
\end{align*}
\]

See (Bauschke et al., 2011) Section 16 for the proof.

For convex set \( C \subset \mathbb{R}^m \), the relative interior of \( C \) is defined by

\[
\text{relint}(C) := \{ v \in C \mid \forall w \in C : \exists \epsilon > 0 \text{ s.t. } v + \epsilon(w - v) \in C \}.
\]

2.2. Problem Formulation

In this study, we consider an optimization problem, formulated as

\[
\min_{\beta \in \mathbb{R}^d} f(X\beta) + g(\beta),
\]

(2)
where \( \beta \in \mathbb{R}^d \) is the optimization variable, \( X \in \mathbb{R}^{n \times d} \) is a constant matrix, and \( f : \mathbb{R}^n \to (-\infty, \infty] \) and \( g : \mathbb{R}^d \to (-\infty, \infty] \) are proper lower semicontinuous convex functions. We assume

\[
\exists \beta \in \text{relint}(\text{dom}(g)) \text{ s.t. } X\beta \in \text{relint}(\text{dom}(f))
\]

and the existence of the optimal point, i.e.,

\[
\exists \hat{\beta} \in \text{dom}(P) \text{ s.t. } P(\hat{\beta}) = \inf_{\beta \in \mathbb{R}^d} P(\beta),
\]

where \( P : \mathbb{R}^d \to \mathbb{R} \) is defined as \( P(\beta) = f(X\beta) + g(\beta) \). Note that we have not assumed the uniqueness of the solution. Moreover, we focus on the cases where \( g \) induces sparsity. Although all theorems in this paper hold, we cannot eliminate any variables without sparsity.

This class of optimization problem is popular, the most popular example of which is Lasso (Tibshirani, 1996):

\[
\min_{\beta \in \mathbb{R}^d} \frac{1}{2} \| y - X\beta \|^2_2 + \lambda \| \beta \|_1.
\]

Many extensions of Lasso, including Group-Lasso (Yuan & Lin, 2006), Elastic-Net (Zou & Hastie, 2005), and sparse logistic regression (Meier et al., 2008) are in this class. Note that non-convex extensions such as SCAD (Fan & Li, 2001), Bridge (Frank & Friedman, 1993), and MCP (Zhang et al., 2010) do not satisfy this assumption.

Another example of the problem in Eq. (2) is the dual problem of a support vector machine (SVM) (Cortes & Vapnik, 1995). The dual problem of SVM can be formulated as follows:

\[
\min_{\beta \in \mathbb{R}^d : 0 \leq \beta \leq 1} \frac{1}{2} \| X\beta \|^2_2 - 1^\top \beta.
\]

The dual problem of a support vector regression (SVR) (Smola & Schölkopf, 2004) is also a target problem. Note that we cannot eliminate any variables of the primal problem of the normal SVM and SVR owing to a lack of sparsity. However, screening methods are available for the primal problem of the feature sparse variants of SVM and SVR (Ghaoui et al., 2010; Shibagaki et al., 2016).

2.3. Dual Problem

To derive a safe screening rule for the optimization problem, Eq. (2), the Fenchel-Rockafellar dual formulation, plays an important role.
Theorem 2 (Fenchel-Rockafellar Duality) If all assumptions for the optimization problem (2) are satisfied, we have the following:

\[
\min_{\beta \in \mathbb{R}^d} f(X\beta) + g(\beta) = \max_{\theta \in \mathbb{R}^n} (-f^*(-\theta) - g^*(X^T\theta)). \tag{3}
\]

The proof of Theorem 2 is given in the Appendix. Let us denote \(-f^*(-\theta) - g^*(X^T\theta)\) by \(D(\theta)\). For primal/dual solutions, we know many conditions that are equivalent to the optimality. Herein, we provide a list of such conditions for convenience.

Proposition 3 (Optimal Condition) If all assumptions for the optimization problem (2) are satisfied, the following are equivalent:

(a) \(\hat{\beta} \in \arg\min_{\beta \in \mathbb{R}^d} P(\beta) \land \hat{\theta} \in \arg\max_{\theta \in \mathbb{R}^n} D(\theta)\)

(b) \(P(\hat{\beta}) = D(\hat{\theta})\)

(c) \(f(X\hat{\beta}) + f^*(-\hat{\theta}) = -\hat{\theta}^T X\hat{\beta} = -g(\hat{\beta}) - g^*(X^T\hat{\theta})\)

(d) \(-\hat{\theta} \in \partial f(X\hat{\beta}) \land X^T\hat{\theta} \in \partial g(\hat{\beta})\)

(e) \(X\hat{\beta} \in \partial f^*(-\hat{\theta}) \land \hat{\beta} \in g^*(X^T\hat{\theta})\)

(Proof) (a) \(\iff\) (b) is directly derived from the strong duality. (b) \(\iff\) (c) is derived from the Fenchel-Young inequality (1). (c) \(\iff\) (d) \(\iff\) (e) are derived from Proposition 1.

2.4. Relationship of Dual Safe Region and Screening

In this section, we show that we can eliminate some features by constructing a simple region that contains \(\hat{\theta}\).

Theorem 4 Assume that all assumptions for the optimization problem (2) are satisfied. Let \(\hat{\beta}\) be the primal optimal point. Assume that the dual optimal point \(\hat{\theta}\) is within the region \(\mathcal{R}\). Then,

\[
\hat{\beta} \in \bigcup_{\theta \in \mathcal{R}} \partial g^*(X^T\theta).
\]

(Proof) According to Proposition 3, \(\hat{\beta} \in \partial g^*(X^T\hat{\theta}) \subseteq \bigcup_{\theta \in \mathcal{R}} \partial g^*(X^T\theta)\).

Theorem 4 provides a general method for feature screening. A simple example is the following corollary.

Corollary 5 Consider an optimization problem, i.e., Eq. (2) with \(g(\beta) = ||\beta||_1\). Assume that \(\hat{\theta} \in \mathcal{R}\). We then have

\[
\max_{\theta \in \mathcal{R}} |x_i^T\theta| < 1 \implies \hat{\beta}_i = 0.
\]

(Proof) By definition of \(g\), we have \(\partial g^*(X^T\theta) \subseteq \{\theta \mid \beta_i = 0\} \iff |x_i^T\theta| < 1\). When \(\max_{\theta \in \mathcal{R}} |x_i^T\theta| < 1\), we have \(\beta_i \in \bigcup_{\theta \in \mathcal{R}} \partial g^*(X^T\theta) \subseteq \{\beta \mid \beta_i = 0\}\) by Theorem 4.

Note that the computational cost of \(\bigcup_{\theta \in \mathcal{R}} \partial g^*(X^T\theta)\) depends on the simplicity of \(g\) and \(\mathcal{R}\).

The key challenge of screening is to determine the simple narrow region \(\mathcal{R}\). Many regions have been proposed for various problems. In the next section, we provide a general framework for constructing a safe region.

3. General Framework for Constructing Safe Region

Herein, we propose a general framework for constructing a dual region that has the solution to the optimization problem in Eq. (3). Our framework consists of a general lower bound and a problem adaptive upper-bound of the optimal value. Hence, we can derive a narrower region than the framework with a general upper bound under certain situations. The general lower-bound is given in the next Theorem.

Theorem 6 Consider the optimization problem in Eq. (3) and assume that \(f^*\) is \(L\)-strongly convex \((L \geq 0)\). Let \(\theta\) be the solution to (3). Then, for \(\forall \theta \in \mathbb{R}^n\), we have

\[
l(\theta; \hat{\theta}) \leq D(\hat{\theta}),
\]

where 

\[
l(\theta; \hat{\theta}) = \frac{L}{2} ||\theta - \hat{\theta}||_2^2 + D(\hat{\theta}).
\]

(Proof) According to Proposition 3, \(X\hat{\beta} \in \partial f^*(-\hat{\theta})\) and \(\beta \in \partial g^*(X^T\hat{\theta})\) hold. Because \(f^*\) is \(L\)-strongly convex and \(g^*\) is convex, for \(\forall \theta \in \mathbb{R}^n\), we have

\[
f^*(-\hat{\theta}) + (X\hat{\beta})^T(-\hat{\theta} + \hat{\theta}) + \frac{L}{2} ||\theta - \hat{\theta}||_2^2 \leq f^*(-\hat{\theta}),
\]

\[
g^*(X^T\hat{\theta}) + \hat{\beta}^T(X^T\hat{\theta} - X^T\hat{\theta}) \leq g^*(X^T\hat{\theta}).
\]

Adding these two inequalities, we have the inequality (4).

This means that \(\hat{\theta}\) is within the region of \(\{\theta \mid l(\theta; \hat{\theta}) \leq D(\hat{\theta})\}\). Because this region is too complicated for screening, we use a simple upper bound of \(D(\theta)\) to construct a simple safe region. The next theorem can be directly derived from Theorem 6.

Theorem 7 Consider the optimization problem in Eq. (3) and assume that \(f^*\) is \(L\)-strongly convex \((L \geq 0)\). Let \(\theta\) be the solution to Eq. (3). Assume \(D(\theta)\) is upper bounded by \(u(\theta)\), i.e., \(\forall \theta \in \mathbb{R}^n\) \(D(\theta) \leq u(\theta)\). Then, for \(\forall \theta \in \mathbb{R}^n\), we have

\[
\hat{\theta} \in \mathcal{R}(\hat{\theta}, u) = \{\theta \mid l(\theta; \hat{\theta}) \leq u(\theta)\}.
\]
The complexity of $\mathcal{R}(\hat{\theta}, u)$ depends on the complexity of $u$. For example, if $u$ is linear, then $\mathcal{R}(\hat{\theta}, u)$ is a sphere. We can construct a narrow, simple, and safe region with a tight simple upper-bound $u$.

In fact, the Gap Safe Sphere region (Fercoq et al., 2015; Ndiaye et al., 2017) can be derived easily from this theorem and weak duality.

**Corollary 8 (Gap Safe Sphere)** Consider the optimization problem in Eq. (3) and assume that $f^*$ is $L$-strongly convex ($L \geq 0$). Let $\hat{\theta}$ be the solution to Eq. (3). For $\forall \tilde{\beta} \in \mathbb{R}^d$ and $\forall \theta \in \mathbb{R}^n$, the region of the Gap Safe Sphere is given as

$$\mathcal{R}^GS(\tilde{\beta}, \hat{\theta}) = \{ \theta \mid l(\theta; \hat{\theta}) \leq P(\tilde{\beta}) \}. \quad (5)$$

Then,$$
\hat{\theta} \in \mathcal{R}^GS(\tilde{\beta}, \hat{\theta}).
$$

**(Proof)** Based on a weak duality, we have $\forall \theta \ D(\theta) \leq P(\tilde{\beta})$. Using this constant function as an upper bound in Theorem 7, the corollary is derived directly. □

Hence, our framework can be seen as a generalization of Gap Safe. Owing to this generalization, we can use a stronger problem-adaptive upper-bound than a weak duality. In the next section, we derive specific regions for Lasso-like problem. Some regions for other problems are given in the Appendix.

### 4. Safe region for Lasso-like problem

In this section, we introduce a strong upper bound for the dual problems of Lasso and similar problems. The dome region derived from it can be seen as a generalization of Sasvi (Liu et al., 2014) and is narrower than Gap Safe Sphere and Gap Safe Dome.

#### 4.1. Norm-regularized least squares problem and its generalization

Norm-regularized least squares is an optimization problem and is formulated as

$$\text{minimize}_{\beta \in \mathbb{R}^d} \frac{1}{2} \| y - X\beta \|_2^2 + g(\beta)$$

where $g$ is a norm. Apparently, this is a subset of problems 2. Although this formulation includes Lasso (Tibshirani, 1996), (overlapping) group-Lasso (Yuan & Lin, 2006; Jacob et al., 2009), and ordered weighted L1 regression (Figueiredo & Nowak, 2016), the non-negative Lasso is not included. To unify them, we define the Lasso-like problem as follows:

$$\text{minimize}_{\beta \in \mathbb{R}^d} \frac{1}{2} \| y - X\beta \|_2^2 + g(\beta), \quad (6)$$

where the problem satisfies all assumptions for Eq. (2) and $g$ satisfies

$$\forall k \geq 0, \beta \in \mathbb{R}^d \quad g(k\beta) = kg(\beta). \quad (7)$$

For the Lasso-like problem, the Fenchel conjugate function of $f$ and $g$ are given as

$$f^*(-\theta) = \frac{1}{2} \| \theta \|_2^2 - y^\top \theta, \quad (8)$$

$$g^*(X^\top \theta) = \begin{cases} 0 & (\forall \beta \quad \theta^\top X\beta - g(\beta) \leq 0) \\ \infty & (\exists \beta \quad \theta^\top X\beta - g(\beta) > 0). \end{cases} \quad (9)$$

Note that $\{ \theta \mid g^*(X^\top \theta) = 0 \}$ is a closed convex set. Hence, the Lasso-like problem is a class of problems whose Fenchel-Rockafellar dual can be seen as a convex projection.

#### 4.2. Proposed Dome Region for Lasso-like problem

Thanks to Theorem 6, we can construct a safe region by proposing an upper bound $u(\theta)$. In this section, we propose a tight upper bound for Lasso-like problems.

The direct expression of $f^*$ in Eq. (8) is sufficiently simple. We only need an upper bound of $-g^*$ to construct a simple region. The upper bound is given as follows:

**Lemma 9** For Lasso-like problems (6), for $\forall \tilde{\beta} \in \mathbb{R}^d$ and $\forall \theta \in \mathbb{R}^n$, we have

$$-g^*(X^\top \theta) \leq \inf_{k \geq 0} g(k\tilde{\beta}) - \theta^\top X(k\tilde{\beta}) \leq \begin{cases} 0 & (g(\tilde{\beta}) - \theta^\top X\tilde{\beta} \geq 0) \\ \infty & (g(\tilde{\beta}) - \theta^\top X\tilde{\beta} < 0). \end{cases} \quad (10)$$

**(Proof)** Based on a Fenchel-Young inequality (1), we have

$$-g^*(X^\top \theta) \leq \inf_{k \geq 0} g(k\tilde{\beta}) - \theta^\top X(k\tilde{\beta}).$$

Under the condition of Eq. (7), we have $g(k\tilde{\beta}) = kg(\tilde{\beta})$. Therefore, the optimal value of the upper bound is zero if $g(\tilde{\beta}) - \theta^\top X(\tilde{\beta}) \geq 0$ and $-\infty$ otherwise. □

The next theorem can be directly derived from Lemma 9.

**Theorem 10** Consider Lasso-like problems in Eq. (6). Let

$$u^{DS}(\theta; \tilde{\beta}) := \begin{cases} f^*(-\theta) & (g(\tilde{\beta}) - \theta^\top X\tilde{\beta} \geq 0) \\ -\infty & (g(\tilde{\beta}) - \theta^\top X\tilde{\beta} < 0). \end{cases} \quad (11)$$

Then, for $\forall \tilde{\beta} \in \mathbb{R}^d$ and $\forall \theta \in \mathbb{R}^n$,

$$D(\theta) \leq u^{DS}(\theta; \tilde{\beta}).$$

Then, Theorem 7 provides a simple and safe region.
Theorem 11 Consider the Lasso-like problem in Eq. (6) and its Fenchel-Rockafellar dual problem in Eq. (3). Let $\hat{\theta}$ be the dual optimal point. We assume that $\hat{\beta} \in \mathbb{R}^d$ and $\theta \in \text{dom}(D)$. Then, $\hat{\theta}$ is within the Dynamic Sasvi region, which is given as an intersection of a sphere and a half space:

$$
\mathcal{R}^{DS}(\hat{\beta}, \hat{\theta}) := \{ \theta \mid l(\theta, \hat{\theta}) \leq u^{DS}(\theta, \hat{\beta}) \},
$$

$$
\{ \theta \mid \left\| \theta - \frac{1}{2} \tilde{\theta} + y \right\|^2 \leq \frac{1}{4} \left\| \tilde{\theta} - y \right\|^2 \wedge 0 \leq g(\hat{\beta}) - \theta^T X \hat{\beta} \}.
$$

The proof of Theorem 11 is given in the Appendix. Because of continuity, $\mathcal{R}^{DS}(\hat{\beta}^{(t)}, \hat{\theta}^{(t)})$ converges to $\mathcal{R}^{DS}(\hat{\beta}, \hat{\theta}) = \{ \theta \}$ if $\lim_{t \to \infty} \hat{\beta}^{(t)} = \hat{\beta}$ and $\lim_{t \to \infty} \hat{\theta}^{(t)} = \hat{\theta}$ hold.

4.3. Relation to Sasvi

In this section, we show that safe screening with variational inequality (Sasvi) (Liu et al., 2014) is a special case of our screening rule. First, we review Sasvi. The target task of Sasvi is to minimize $\frac{1}{2} \|y - X\beta\|^2 + \lambda \|\beta\|$ with many $\lambda$s. Divided by $\lambda^2$ and change optimization variable, we obtain the following:

$$
\min_{\beta \in \mathbb{R}^d} \frac{1}{\lambda} \left\| y - X\beta \right\|^2_2 + \left\| \beta \right\|_1.
$$

Let $\hat{\beta}^{(\lambda)}$ and $\hat{\theta}^{(\lambda)}$ be the optimal points of the primal problem and the Fenchel-Rockafellar dual problem, respectively. Sasvi uses $\hat{\theta}^{(\lambda_0)}$ to construct a safe region for $\hat{\theta}^{(\lambda)}$. Although Sasvi was originally proposed for Lasso, it can be easily generalized for the Lasso-like problem as follows.

Theorem 12 Let $\hat{\theta}^{(\lambda)}$ be the optimal point of the Fenchel-Rockafellar dual problem of the Lasso-like problem (that is, $g$ satisfies Eq. (7))

$$
\max_{\theta, g^*(X^T \theta) = 0} \left( \frac{1}{\lambda} \left\| y - \theta \right\|^2_2 + \frac{1}{2} \left\| \frac{1}{\lambda} y \right\|^2_2 \right).
$$

Assume we have an exact $\hat{\theta}^{(\lambda_0)}$. We then have

$$
\hat{\beta}^{(\lambda)} \in \mathcal{R}^{\text{Sasvi}}(\lambda, \lambda_0) := \{ \theta \mid 0 \geq \left( \frac{1}{\lambda} y - \theta \right)^T \left( \hat{\theta}^{(\lambda_0)} - \theta \right) \wedge 0 \geq \left( \frac{1}{\lambda_0} y - \hat{\theta}^{(\lambda_0)} \right)^T \left( \theta - \hat{\theta}^{(\lambda_0)} \right) \}
$$

(Proof) Because the duality of the Lasso-like problem can be interpreted as a projection from $\frac{1}{\lambda} y$ to a closed convex set $\{ \theta \mid g^*(X^T \theta) = 0 \}$, two variational inequalities hold. See (Liu et al., 2014) for more details.

We can then prove that $\mathcal{R}^{\text{Sasvi}}(\lambda_0) := \mathcal{R}^{\text{Sasvi}}(1, \lambda_0)$ equals $\mathcal{R}^{DS}(\hat{\beta}^{(\lambda_0)}, \hat{\theta}^{(\lambda_0)})$. Note that we can set $\lambda = 1$ without a loss of generality because multiplying the same scalar to $y$, $\lambda$, and $\lambda_0$ does not change the problem or the region.

Theorem 13 Consider the Lasso-like problem

$$
\min_{\beta \in \mathbb{R}^d} \frac{1}{\lambda} \left\| y - X\beta \right\|^2_2 + g(\beta).
$$

Let $\hat{\beta}^{(\lambda)}$ and $\hat{\theta}^{(\lambda)}$ be the primal/dual optimal points, respectively. We then have

$$
\mathcal{R}^{\text{Sasvi}}(\lambda_0) = \mathcal{R}^{DS}(\hat{\beta}^{(\lambda_0)}, \hat{\theta}^{(\lambda_0)}),
$$

where $\mathcal{R}^{\text{Sasvi}}(\lambda_0)$ and $\mathcal{R}^{DS}(\hat{\beta}^{(\lambda_0)}, \hat{\theta}^{(\lambda_0)})$ are safe regions for $\hat{\theta}^{(1)}$.

The proof of Theorem 13 is given in the Appendix. For this reason, we have labeled it "Dynamic Sasvi." This generalization increases the speed of the solver significantly because the region of our method may be extremely narrow in the late stage of optimization. As pointed out in (Fercoq et al., 2015), some sequential safe screening rules, including Sasvi, are not safe in practice because we do not have the exact solution for $\lambda_0$. Dynamic Sasvi overcomes this problem because its region is safe if it is not the exact solution.

4.4. Comparison to Gap Safe Dome and Gap Safe Sphere

Here, we show that the proposed method is stronger than Gap Safe Dome (Fercoq et al., 2015) and Gap Safe Sphere (Fercoq et al., 2015), (Ndiaye et al., 2017) for Lasso-like problems. As shown in (Fercoq et al., 2015), for Lasso, the regions of the Gap Safe Dome and Gap Safe Sphere are the relaxation of the intersection of a sphere and the contra of another sphere. We call this unrelaxed region Gap Safe Moon. Although Gap Safe Moon is defined only for Lasso in (Fercoq et al., 2015), it can be naturally generalized for Lasso-like problems. Gap Safe Moon can be derived from Corollary 7.

Theorem 14 (Gap Safe Moon) Consider the Lasso-like problem in Eq. (6) and its dual Fenchel-Rockafellar equation, i.e., Eq. (3). Let $\hat{\theta}$ be the dual optimal point. For $\hat{\beta} \in \mathbb{R}^d$, the Gap Safe Moon upper bound is given as

$$
\mathbf{u}^{GM}(\theta; \hat{\beta}) = \begin{cases}
-f^*(-\theta) & \text{if } -f^*(-\theta) \leq P(\hat{\beta}) \\
\infty & \text{if } -f^*(-\theta) > P(\hat{\beta})
\end{cases}.
$$

Then, for $\forall \hat{\beta} \in \mathbb{R}^d$, $\forall \hat{\theta} \in \text{dom}(D)$, and $\forall \theta \in \mathbb{R}^n$, we have $D(\theta) \leq \mathbf{u}^{GM}(\theta; \hat{\beta})$. 
This theorem means that the region of dynamic Sasvi is a minimum radius sphere that includes the dynamic Sasvi region. Figure 1b shows the regions of Dynamic Sasvi, Gap Safe Moon and Dynamic Sasvi. For \( \beta \in \mathbb{R}^d \) and \( \theta \in \mathbb{R}^n \), we have
\[
u^{\text{DS}}(\theta; \beta) \leq u^{\text{GM}}(\theta; \hat{\beta}).
\]

**Theorem 15 (Gap Safe Moon and Dynamic Sasvi)** For all \( \beta \in \mathbb{R}^d \) and all \( \theta \in \mathbb{R}^n \), we have
\[
u^{\text{DS}}(\theta; \beta) \leq u^{\text{GM}}(\theta; \hat{\beta}).
\]

**Theorem 16** Consider the Lasso-like problem in Eq. (6) and its Fenchel-Rockafellar dual problem in Eq. (3). We assume that \( \hat{\beta} \in \mathbb{R}^d \) and \( \hat{\theta} \in \text{dom}(D) \). If \( n \geq 2 \), the minimum radius sphere including \( R^{\text{DS}}(\beta, \hat{\theta}) \) is
\[
R^{\text{DE}}(\hat{\beta}, \hat{\theta}) = \{ \theta \mid \|\theta - \theta_c\|_2^2 \leq r^2 \},
\]
where
\[
\theta_c = \frac{1}{2} (\hat{\beta} + y) - \alpha X \hat{\beta},
\]
\[
r^2 = \frac{1}{4} \|\hat{\beta} - y\|_2^2 - \alpha^2 \|X \hat{\beta}\|_2^2
\]
\[
\alpha = \max \left( 0, \frac{1}{\|X \beta\|_2^2 - \frac{1}{2} (\hat{\theta} + y)^T (\hat{\theta} - \hat{\beta}) \} \right).
\]

The proof of Theorem 16 is given in the Appendix. Figures 1a and 1c show the dynamic EDPP region and other regions. Note that the dynamic EDPP region is not guaranteed to be within the Gap Safe Sphere region. However, its radius is always smaller than that of Gap Safe Sphere.

5. Implementation for Lasso

In this section, we provide a specific solver based on Theorem 11. Because the algorithm used to calculate \( \bigcup_{\theta \in \mathbb{R}^n} \partial g^*(X^T \theta) \) depends on \( g \), we introduce a Lasso solver as an example. We must choose an iterative solver to combine with screening methods because they cannot estimate the solution alone. Although our methods can work with any iterative method, we use coordinate descent, which is recommended in (Friedman et al., 2007).

5.1. Choice of \( \hat{\theta} \)

As shown in the previous section, \( \lim_{t \to \infty} R^{\text{DS}}(\beta^t, \theta^t) \) converges to \( \{ \hat{\theta} \} \) when \( \lim_{t \to \infty} \theta^t = \beta \) and \( \lim_{t \to \infty} \theta^t = \hat{\theta} \) holds. Because the iterative solver provides such a sequence of primal points and screening does not harm its
Algorithm 1 Coordinate descent with Dynamic Sasvi for Lasso

1: Input: \( X, y, \beta_0, T, c, \epsilon \)
2: Initialize \( \beta \leftarrow \beta_0, A \leftarrow [d] \)
3: for \( t \in [T] \) do
4: if \( k \mod c = 1 \) then
5: Compute \( \hat{\beta} = \psi_A(\beta) \)
6: if \( P(\beta) - D(\hat{\beta}) \leq c \) then
7: break
8: end if
9: \( \mathcal{R} \leftarrow \mathcal{R}^{DS}(\hat{\beta}, \hat{\theta}) \)
10: \( A \leftarrow \{ j \in A : \max_{\theta \in \mathcal{R}} |x_j^\top \theta| \geq 1 \} \)
11: for \( j \in [d] - A \) do
12: \( \beta_j \leftarrow 0 \)
13: end for
14: end if
15: for \( j \in A \) do
16: \( u \leftarrow \hat{\beta}_j \|x_j\|_2^2 - x_j^\top (X \hat{\beta} - y) \)
17: \( \tilde{\beta}_j \leftarrow \frac{1}{\|x_j\|_2} \text{sign}(u) \max(0, |u| - 1) \)
18: end for
19: end for
20: Output: \( \hat{\beta} \)

Now, we can optimize the problem with the proposed screening. The pseudo code is described in Algorithm 1. Direct expression of \( \max_{\theta \in \mathcal{R}^{DS}(\hat{\beta}, \hat{\theta})} |x_j^\top \theta| \) is given in the Appendix.

5.2. Computational Cost of Dynamic Sasvi Screening

In Dynamic Sasvi screening, the calculation of \( \phi_A(\hat{\beta}) \) and \( \max_{\theta \in \mathcal{R}} |x_j^\top \theta| \) controls the computational cost. If we have \( X \hat{\beta}, X^\top X \hat{\beta} \), and \( X^\top y \), we can obtain \( \phi_A(\beta) \) with \( O(n + d) \) calculations. If we have \( X \hat{\beta}, X^\top X \hat{\beta}, \hat{\theta}, X^\top \hat{\theta}, \) and \( X^\top y \), we can obtain \( \max_{\theta \in \mathcal{R}} |x_j^\top \theta| \) for all \( j \) with \( O(n + d) \) calculations. Because \( X^\top y \) is constant and \( \hat{\theta} = \phi_A(\beta) \) is a linear combination of \( X \hat{\beta} \) and \( y \), the calculations of only \( X \hat{\beta} \) and \( X^\top X \hat{\beta} \) cost \( O(nd) \). Hence, the screening cost is almost the same for all methods, which require \( X^\top X \hat{\beta} \), including Gap Safe.

5.3. Computation of Lasso Path

In practice, we formulate the Lasso problem as follows:

\[
\minimize_{\beta \in \mathbb{R}^d} \frac{1}{2} \| y - X \beta \|_2^2 + \|\beta\|_1
\]

and solve for many values of \( \lambda \) to choose the best solution. Considering the situation in which we have to estimate the solutions \( \beta^{(\lambda_1)}, \beta^{(\lambda_2)}, \ldots, \beta^{(\lambda_M)} \) corresponds to \( \lambda_1 > \lambda_2 > \cdots > \lambda_M \). Many studies (e.g., (Fercoq et al., 2015)) recommend using the estimated solution for \( \lambda_{m-1} \) as the initial vector in the estimation of \( \beta^{(\lambda_m)} \) because \( \beta^{(\lambda_{m-1})} \) and \( \beta^{(\lambda_m)} \) may be close. In our implementation, we set the initial vector as \( k \beta^{(\lambda_{m-1})} \), where \( \beta^{(\lambda_{m-1})} \) is the estimation of \( \beta^{(\lambda_{m-1})} \) and

\[
k := \argmin_{k \geq 0} \frac{1}{2} \| \frac{1}{\lambda_m} y - k X \beta^{(\lambda_{m-1})} \|_2^2 + k \|\beta^{(\lambda_{m-1})}\|_1
\]

6. Experiments

In this section, we show the efficacy of the proposed methods using real-world data.

6.1. Setup

We compared the proposed methods with Gap Safe Sphere and Gap Safe Dome (Fercoq et al., 2015; Ndiaye et al., 2017), which are state-of-the-art dynamic safe screening methods. All methods were run on a Macbook Air with a 1.1 GHz quad-core Intel Core i5 CPU with 16 GB of RAM. We implemented all methods in C++ using the Accelerate framework, which is the native framework for basic calculations.

convergence, we only need a converging sequence of dual points to obtain a converging safe region. The next theorem presents such a sequence.

**Theorem 17 (Converging \( \theta' \))** Consider the optimization problem Eq. (6) with \( g(\beta) = \|\beta\|_1 \). Let \( \hat{\beta} \in \mathbb{R}^d \) and \( \theta \in \mathbb{R}^n \) be the primal/dual solution. Assume \( \lim_{t \to \infty} \beta^t = \hat{\beta} \). Let us define \( \phi : \mathbb{R}^d \to \mathbb{R}^n \) as

\[
\phi(\beta) := \frac{1}{\max(1, \|X^\top(y - X \beta)\|_{\infty})} (y - X \beta).
\]

Then, \( \forall \beta, \phi(\beta) \in \text{dom}(D) \) and \( \lim_{t \to \infty} \phi(\beta^t) = \hat{\theta} \) hold.

**Proof** \( \phi(\beta) \in \text{dom}(D) \) is directly derived from \( \|X^\top \phi(\beta)\|_{\infty} = \min(\|X^\top(y - X \beta)\|_{\infty}, 1) \leq 1 \). Because \( \phi \) is continuous and \( \phi(\hat{\beta}) = \hat{\theta} \), \( \lim_{t \to \infty} \phi(\beta^t) = \hat{\theta} \) also holds.

Actually, if \( A \) is the set of features that is not yet eliminated, we can use

\[
\phi_A(\beta) := \frac{1}{\max(1, \max_{j \in A} |x_j(y - X \beta)|)} (X \beta - y)
\]

instead of \( \phi(\beta) \). Although \( \phi_A(\beta) \in \text{dom}(D) \) is not guaranteed, \( \phi_A(\beta) \) is guaranteed to satisfy all constraints that are active in the dual solution. In other words, \( \phi_A(\beta) \) is in the domain of the dual problem of the small primal problem without eliminated features.
6.2. Number of screened variables

First, we compared the number of screened variables among the four dynamic safe screening methods. We solved the Lasso problem using the Leukemia dataset (dense data with 72 samples and 7128 features) and \( \lambda = \frac{1}{\mathbf{1}^\top \mathbf{X}^\top \mathbf{y}} \). We used cyclic coordinate descent as the iterative algorithm and screen variables for 10 iterations each. Figure 2a shows the ratio of the uneliminated features at each iteration. As guaranteed theoretically, we can see that Dynamic Sasvi eliminates more variables in earlier steps than Gap Safe Dome and Gap Safe Sphere. The figure also shows that Dynamic EDPP, relaxed version of Dynamic Sasvi, eliminated almost the same number of features as Dynamic Sasvi.

6.3. Gains in the computation of Lasso paths

Next, we compared the computation time of the path of the Lasso solutions for various values of \( \lambda \). Because \( \lambda \) may be defined by a cross validation in practice, computing the path of the solutions is an important task. We used \( \lambda_j = 100^{-\log \epsilon} \| \mathbf{X}^\top \mathbf{y} \|_\infty \) (\( j = 0, \ldots, 99 \)). The iterative solver stops when the duality gap is smaller than \( \epsilon (P(0) - D(0)) \). Note that \( P(0) - D(0) \) makes the stopping criterion independent of the data scale. We used the Leukemia and tf-idf vectorized 20newsgroup datasets (baseball versus hockey) (sparse data with 1197 samples and 18571 features). We subsampled the data 50 times and ran all methods for the same 50 subsamples. The subsampled data size is 50 for leukemia and 800 for 20newsgroup. Figures 2b and 2c show the average computation time of the Lasso path for the Leukemia dataset and 20news datasets, respectively. For all settings, dynamic Sasvi and dynamic EDPP outperform Gap Safe Dome and Gap Safe Sphere.

Table 1 shows the the average and standard deviations of the logarithm of the acceleration ratio to the computational time for the same subsample without screening. Proposed methods are significantly faster than Gap Safe methods. In addition, Dynamic EDPP is a little faster than Dynamic Sasvi because the computational cost of Dynamic EDPP screening is smaller than the one of Dynamic Sasvi.

7. Conclusion

In this paper, we proposed a framework for safe screening based on Fenchel-Rockafellar duality and derived Dynamic Sasvi and Dynamic EDPP, which are specific safe screening methods for Lasso-like problems. Dynamic Sasvi and Dynamic EDPP can be regarded as dynamic feature elimination variants of Sasvi and EDPP, respectively. We proved that Dynamic Sasvi always eliminates more features than Gap Safe Sphere and Gap Safe Dome. Dynamic EDPP is based on the sphere relaxation of the Dynamic Sasvi region and eliminates almost the same number of features as Dynamic Sasvi. We also showed experimentally that the computational costs of the proposed methods are smaller than those of Gap Safe Sphere and Gap Safe Dome.
References

Bao, R., Gu, B., and Huang, H. Fast oscar and owl regression via safe screening rules. In ICML, 2020.

Bauschke, H. H., Combettes, P. L., et al. Convex analysis and monotone operator theory in Hilbert spaces, volume 408. Springer, 2011.

Bonnefoy, A., Emiya, V., Ralaivola, L., and Gribonval, R. Dynamic screening: Accelerating first-order algorithms for the lasso and group-lasso. IEEE Transactions on Signal Processing, 63(19):5121–5132, 2015.

Climente-Gonz´alez, H., Azencott, C.-A., Kaski, S., and Yamada, M. Block hsic lasso: model-free biomarker detection for ultra-high dimensional data. Bioinformatics, 35(14):i427–i435, 2019.

Cortes, C. and Vapnik, V. Support-vector networks. Machine learning, 20(3):273–297, 1995.

Donoho, D. L. Compressed sensing. IEEE Transactions on information theory, 52(4):1289–1306, 2006.

Fan, J. and Li, R. Variable selection via nonconcave penalized likelihood and its oracle properties. Journal of the American statistical Association, 96(456):1348–1360, 2001.

Fercoq, O., Gramfort, A., and Salmon, J. Mind the duality gap: safer rules for the lasso. In ICML, 2015.

Figueiredo, M. and Nowak, R. Ordered weighted l1 regularized regression with strongly correlated covariates: Theoretical aspects. In AISTATS, 2016.

Frank, L. E. and Friedman, J. H. A statistical view of some chemometrics regression tools. Technometrics, 35(2):109–135, 1993.

Friedman, J., Hastie, T., Höfling, H., and Tibshirani, R. Pathwise coordinate optimization. Ann. Appl. Stat., 1(2):302–332, 12 2007.

Ghaoui, L. E., Viallon, V., and Rabbani, T. Safe feature elimination for the lasso and sparse supervised learning problems. arXiv preprint arXiv:1009.4219, 2010.

Jacob, L., Obozinski, G., and Vert, J.-P. Group lasso with overlap and graph lasso. In ICML, 2009.

Liu, J., Zhao, Z., Wang, J., and Ye, J. Safe screening with variational inequalities and its application to lasso. In ICML, 2014.

Meier, L., Van De Geer, S., and Bühlmann, P. The group lasso for logistic regression. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 70(1): 53–71, 2008.

Ndiaye, E., Fercoq, O., Gramfort, A., and Salmon, J. Gap safe screening rules for sparse multi-task and multi-class models. In NIPS, 2015.

Ndiaye, E., Fercoq, O., Gramfort, A., and Salmon, J. Gap safe screening rules for sparsity enforcing penalties. Journal of Machine Learning Research, 18(1):4671–4703, 2017.

Ndiaye, E., Fercoq, O., and Salmon, J. Screening rules and its complexity for active set identification, 2020.

Ogawa, K., Suzuki, Y., and Takeuchi, I. Safe screening of non-support vectors in pathwise svm computation. In ICML, 2013.

Raj, A., Olbrich, J., Gärtner, B., Schölkopf, B., and Jaggi, M. Screening rules for convex problems. arXiv preprint arXiv:1609.07478, 2016.

Shibagaki, A., Karasuyama, M., Hatano, K., and Takeuchi, I. Simultaneous safe screening of features and samples in doubly sparse modeling. In ICML, 2016.

Smola, A. J. and Schölkopf, B. A tutorial on support vector regression. Statistics and computing, 14(3):199–222, 2004.

Tibshirani, R. Regression shrinkage and selection via the lasso. Journal of the Royal Statistical Society: Series B (Methodological), 58(1):267–288, 1996.

Wang, J., Wonka, P., and Ye, J. Lasso screening rules via dual polytope projection. Journal of Machine Learning Research, 16(1):1063–1101, 2015.

Xiang, Z. J., Wang, Y., and Ramadge, P. J. Screening tests for lasso problems. IEEE Transactions on Pattern Analysis and Machine Intelligence, 39(5):1008–1027, May 2017.

Yuan, M. and Lin, Y. Model selection and estimation in regression with grouped variables. Journal of the Royal Statistical Society Series B, 68:49–67, 02 2006.

Zhang, C.-H. et al. Nearly unbiased variable selection under minimax concave penalty. The Annals of statistics, 38(2): 894–942, 2010.

Zou, H. and Hastie, T. Regularization and variable selection via the elastic net. Journal of the royal statistical society: series B (statistical methodology), 67(2):301–320, 2005.
A. Proof of Theorems

A.1. Proof of Theorem 2

(Proof) According to ((Bauschke et al., 2011) Theorem 15.23), since we have assumed that

\[ \exists \beta \in \text{relint}(\text{dom}(g)) \text{ s.t. } X\beta \in \text{relint}(\text{dom}(f)), \]

i.e., \( \text{relint}(\text{dom}(f)) \cap X \text{relint}(\text{dom}(g)) \) is not empty, we have

\[ \inf_{\beta \in \mathbb{R}^d} f(X\beta) + g(\beta) = \max_{\theta \in \mathbb{R}^n} -f^*(-\theta) - g^*(X^T \theta). \]

In addition, we have assumed the existence of the optimal point. Hence, we have

\[ \min_{\beta \in \mathbb{R}^d} f(X\beta) + g(\beta) = \max_{\theta \in \mathbb{R}^n} -f^*(-\theta) - g^*(X^T \theta). \]

\[ \Box \]

A.2. Proof of Theorem 11

(Proof) According to Theorem 7, we can easily obtain

\[ \hat{\theta} \in \mathcal{R}^{\text{DS}}(\hat{\beta}, \hat{\theta}) := \{ \theta \mid l(\theta; \hat{\theta}) \leq u^{\text{DS}}(\theta; \hat{\beta}) \}. \]

By the definition of \( u^{\text{DS}} \), we have the following:

\[ l(\theta; \hat{\theta}) \leq u^{\text{DS}}(\theta; \hat{\beta}) \iff l(\theta; \hat{\theta}) \leq -f^*(-\theta) \land 0 \leq g(\hat{\beta}) - \theta^T X \hat{\beta}. \]

In addition, by Eqs. (8), \( g^*(X^T \hat{\theta}) = 0 \) and \( L = 1 \), we have

\[ l(\theta; \hat{\theta}) \leq -f^*(-\theta) \iff \frac{1}{2} \| \theta - \hat{\theta} \|^2_2 - \frac{1}{2} \| \hat{\theta} \|^2_2 + y^T \hat{\theta} \leq -\frac{1}{2} \| \theta \|^2_2 + y^T \theta \]

\[ \iff \| \theta \|^2_2 - \theta^T (\theta + y) \leq -y^T \hat{\theta} \]

\[ \iff \| \theta - \frac{1}{2} (\theta + y) \|^2_2 \leq \frac{1}{4} \| (\theta - y) \|^2_2. \]

Hence, we have

\[ \hat{\theta} \in \mathcal{R}^{\text{DS}}(\hat{\beta}, \hat{\theta}) := \{ \theta \mid l(\theta; \hat{\theta}) \leq u^{\text{DS}}(\theta; \hat{\beta}) \} = \{ \theta \mid \| \theta - \frac{1}{2} (\theta + y) \|^2_2 \leq \frac{1}{4} \| (\theta - y) \|^2_2 \land 0 \leq g(\hat{\beta}) - \theta^T X \hat{\beta} \}. \]

\[ \Box \]

A.3. Proof of Theorem 13

(Proof) First, we prove \( g(\hat{\beta}^{(\lambda_0)}) = \hat{\theta}^{(\lambda_0)}^T X \hat{\beta}^{(\lambda_0)} \). Because \( X^T \hat{\theta}^{(\lambda_0)} \in \partial g(\hat{\beta}^{(\lambda_0)}) \) (Proposition 3), for \( \forall \beta \), the inequality

\[ g(\hat{\beta}^{(\lambda_0)}) + \hat{\theta}^{(\lambda_0)}^T X (\beta - \hat{\beta}^{(\lambda_0)}) \leq g(\beta) \]

holds. We can set \( \beta = 0 \) and \( \beta = 2\hat{\beta}^{(\lambda_0)} \) and obtain

\[ g(\hat{\beta}^{(\lambda_0)}) - \hat{\theta}^{(\lambda_0)}^T X \hat{\beta}^{(\lambda_0)} \leq 0 \]

\[ g(\hat{\beta}^{(\lambda_0)}) + \hat{\theta}^{(\lambda_0)}^T X \hat{\beta}^{(\lambda_0)} \leq 2g(\hat{\beta}^{(\lambda_0)}). \]

Hence, we have \( g(\hat{\beta}^{(\lambda_0)}) = \hat{\theta}^{(\lambda_0)}^T X \hat{\beta}^{(\lambda_0)} \).

In addition, \( \theta^{(\lambda_0)} = \frac{1}{\lambda_0} u - X \hat{\beta}^{(\lambda_0)} \) holds (Proposition 3).
We then have
\[ R_{\text{DS}}(\hat{\beta}(\lambda_0), \tilde{\beta}(\lambda_0)) = \{ \theta \mid \| \theta - \frac{1}{2}(\hat{\beta}(\lambda_0) + y) \|^2 \leq \frac{1}{4} \| (\hat{\beta}(\lambda_0) - y) \|^2 \land 0 \leq g(\hat{\beta}(\lambda_0)) - \theta^\top X\hat{\beta}(\lambda_0) \} \]
\[ = \{ \theta \mid \| \theta \|^2_2 - \theta^\top (\hat{\beta}(\lambda_0) + y) + \frac{1}{4} \| (\hat{\beta}(\lambda_0) + y) \|^2 \leq \frac{1}{4} \| (\hat{\beta}(\lambda_0) - y) \|^2 \land 0 \leq (\hat{\beta}(\lambda_0) - \theta) \top X\hat{\beta}(\lambda_0) \} \]
\[ = \{ \theta \mid \| \theta \|^2_2 - \theta^\top (\hat{\beta}(\lambda_0) + y) + y \top \hat{\beta}(\lambda_0) \leq 0 \land 0 \leq (\hat{\beta}(\lambda_0) - \theta) \top (\frac{1}{\lambda_0} y - \hat{\beta}(\lambda_0)) \} \]
\[ = \{ \theta \mid (y - \theta)^\top (\hat{\beta}(\lambda_0) - \theta) \leq 0 \land \frac{1}{\lambda_0} y - \hat{\beta}(\lambda_0) \leq (\hat{\beta}(\lambda_0) - \theta) \top y \leq 0 \} \]
\[ = R_{\text{Sasvi}}(1, \lambda_0) = R_{\text{Sasvi}}(\lambda_0) \]

A.4. Proof of Theorem 14

(Proof) By Eq. (9), we have \( D(\theta) \in \{ -\infty, -f^*(-\theta) \} \). Clearly, the inequality \( D(\theta) \leq -f^*(-\theta) \) always holds. If \( -f^*(-\theta) > P(\tilde{\beta}) \), \( D(\theta) \) must be \( -\infty \) because \( D(\theta) \leq P(\tilde{\beta}) \). Hence, we have \( D(\theta) \leq u_{\text{GM}}(\theta; \tilde{\beta}) \). According to Theorem 7, we have
\[ \tilde{\theta} \in \{ \theta \mid l(\theta, \tilde{\theta}) \leq u_{\text{GM}}(\theta; \tilde{\beta}) \} \]
\[ = \{ \theta \mid -f^*(-\theta) \leq P(\tilde{\beta}) \land \frac{1}{2} \| \theta - \theta \|^2_2 - f^*(-\theta) - g^*(X^\top \tilde{\theta}) \leq -f^*(-\theta) \} \]
\[ = \{ \theta \mid -f^*(-\theta) \leq P(\tilde{\beta}) \land \frac{1}{2} \| \theta - \theta \|^2_2 - \frac{1}{2} \| \theta \|^2_2 + y \top \theta \leq -\frac{1}{2} \| \theta \|^2 + y \top \theta \} \]
\[ = \{ \theta \mid -f^*(-\theta) \leq P(\tilde{\beta}) \land \| \theta \|^2_2 - \theta^\top y \leq y \top \theta \} \]
\[ = \{ \theta \mid -f^*(-\theta) \leq P(\tilde{\beta}) \land (\hat{\beta} - \theta)^\top (y - \theta) \leq 0 \} \]

A.5. Proof of Theorem 16

Proof of \( R_{\text{DS}}(\tilde{\beta}, \hat{\beta}) \subset R_{\text{DE}}(\tilde{\beta}, \hat{\beta}) \):

(Proof) Since \( \alpha \geq 0 \), we have
\[ R_{\text{DS}}(\tilde{\beta}, \hat{\beta}) = \{ \theta \mid \| \theta - \frac{1}{2}(\hat{\beta} + y) \|^2 \leq \frac{1}{4} \| (\hat{\beta} - y) \|^2 \land 0 \leq g(\hat{\beta}) - \theta^\top X\hat{\beta} \} \]
\[ \subset \{ \theta \mid \| \theta - \frac{1}{2}(\hat{\beta} + y) \|^2 \leq \frac{1}{4} \| (\hat{\beta} - y) \|^2 + 2\alpha (g(\hat{\beta}) - \theta^\top X\hat{\beta}) \} \]
\[ = \{ \theta \mid \| \theta \|^2_2 - \theta^\top (\hat{\beta} + y) + 2\alpha \theta^\top X\hat{\beta} \leq \frac{1}{4} \| (\hat{\beta} - y) \|^2 - \frac{1}{4} \| \theta \|^2_2 + 2\alpha g(\hat{\beta}) \} \]
\[ = \{ \theta \mid \theta - \frac{1}{2}(\hat{\beta} + y) + \alpha X\hat{\beta} \|^2 \leq \frac{1}{4} \| (\hat{\beta} - y) \|^2 - \frac{1}{4} \| \theta \|^2_2 + \frac{1}{2} \| \theta + y \|^2 + \frac{1}{2} \| \hat{\beta} + y \|^2 - \alpha \| X\hat{\beta} \|^2_2 + 2\alpha g(\hat{\beta}) \} \]
\[ = \{ \theta \mid \| \theta - \frac{1}{2}(\hat{\beta} + y) + \alpha X\hat{\beta} \|^2 \leq \frac{1}{4} \| (\hat{\beta} - y) \|^2 + \alpha^2 \| X\hat{\beta} \|^2_2 - 2\alpha (\theta + y)^\top X\hat{\beta} + 2\alpha g(\hat{\beta}) \}. \]

And by \( \alpha \in \{ 0, \frac{1}{\| X\hat{\beta} \|^2_2} \} \), we have
\[ \alpha^2 \| X\hat{\beta} \|^2_2 - (\theta + y)^\top X\hat{\beta} + 2\alpha g(\hat{\beta}) = -\alpha^2 \| X\hat{\beta} \|^2_2. \]
Hence,
\[ \mathcal{R}^{DS}(\beta, \theta) \subseteq \{ \theta \mid \|\theta - \frac{1}{2}(\hat{\theta} + y) + \alpha X \hat{\beta}\|_2^2 \leq \frac{1}{4}\|((\hat{\theta} - y)\|_2^2 - \alpha^2\|X \hat{\beta}\|_2^2 \} \]
\[ = \{ \theta \mid \|\theta - \hat{\theta}\|_2 \leq r^2 \} \]
\[ = \mathcal{R}^{DE}(\beta, \theta) \]
holds.

**Proof of minimality of the radius:**

**(Proof)** Let \( v \in \mathbb{R}^n \) be a vector which satisfies \( v^T X \hat{\beta} = 0 \) and \( v^T v = 1 \). Note that such a vector exists if \( n \geq 2 \). Then, we have \( \theta_c + r v \in \mathcal{R}^{DS}(\beta, \theta) \) because
\[ (\theta_c + r v)^T X \hat{\beta} = \frac{1}{2}(\hat{\theta} + y)^T X \hat{\beta} - \max(0, \frac{1}{2}(\hat{\theta} + y)^T X \hat{\beta} - g(\beta)) \leq g(\beta) \]
and
\[ \|\theta_c + r v - \frac{1}{2}(\hat{\theta} + y)\|_2^2 = \| - \alpha X \hat{\beta} \pm r v\|_2^2 = \frac{1}{4}\|((\hat{\theta} - y)\|_2^2 \]
held. Since the distance between these two points is \( 2r \), the radius of a sphere which includes \( \mathcal{R}^{DS}(\beta, \theta) \) can not be smaller than \( r \).

**B. Direct Expression of** \( \max_{\theta \in \mathcal{R}^{DS}(\beta, \theta)} x^T_j \theta \)

Let \( r = \frac{1}{2}\|\hat{\theta} - y\|_2 \) and \( \theta_o = \frac{1}{2}(\hat{\theta} + y) \).

If \( (\theta_o + \frac{r}{\|x_j\|_2} x_j)^T X \hat{\beta} \leq g(\beta) \), argmax \( \theta \in \mathcal{R}^{DS}(\beta, \theta) \) \( x^T_j \theta = \theta_o + \frac{r}{\|x_j\|_2} x_j \) and max \( \theta \in \mathcal{R}^{DS}(\beta, \theta) \) \( x^T_j \theta = x^T_j \theta_o + r\|x_j\|_2 \).

If \( (\theta_o + \frac{r}{\|x_j\|_2} x_j)^T X \hat{\beta} > g(\beta) \), the constraint \( \theta^T X \hat{\beta} \leq g(\beta) \) guaranteed to be active at the solution. Hence, we have
\[ \max_{\theta \in \mathcal{R}^{DS}(\beta, \theta)} x^T_j \theta = \max_{\|\theta - \theta_o\|_2 \leq r^2} x^T_j \theta \]
\[ = x^T_j \theta_o + \frac{x^T_j X \hat{\beta}}{\|X \hat{\beta}\|_2} (g(\beta) - \theta_o^T X \hat{\beta}) + \max_{\|\theta - \theta_o\|_2 \leq r^2} x^T_j (\frac{X \hat{\beta} - \left( x^T_j X \hat{\beta} \right)_{\|X \hat{\beta}\|_2} X \hat{\beta}}{\|X \hat{\beta}\|_2})^T \theta' \]
\[ = x^T_j \theta_o + \frac{x^T_j X \hat{\beta}}{\|X \hat{\beta}\|_2} (g(\beta) - \theta_o^T X \hat{\beta}) + \frac{1}{\|X \hat{\beta}\|_2} \left( x^T_j X \hat{\beta} - \left( x^T_j X \hat{\beta} \right)_{\|X \hat{\beta}\|_2} X \hat{\beta} \right) \left( \frac{r}{\|x_j\|_2} x^T_j X \hat{\beta} \leq \delta \right) \]
\[ \left( \frac{r}{\|x_j\|_2} x^T_j X \hat{\beta} > \delta \right) \]

**C. Regions for other problems**

According to Theorem 7, we can construct simple safe region by constructing simple upperbound of \( D(\theta) \). Herein, we introduce some regions for non Lasso-like problems.

**Elastic-Net:** Consider the following problem:

\[ \min_{\beta \in \mathbb{R}^d} \frac{1}{2}\|y - X \beta\|_2^2 + g(\beta) \]
where $g(\beta) = \|\beta\|_1 + \frac{\gamma}{2} \|\beta\|_2^2$ and $\gamma > 0$. Then, for $\forall \tilde{\beta}$, we have

$$-g^*(X^\top \theta) \leq \inf_{k \geq 0} g(k\tilde{\beta} - \theta^\top X(k\tilde{\beta}))$$

$$= \inf_{k \geq 0} k(\|\tilde{\beta}\|_1 - \theta^\top X\tilde{\beta}) + \frac{\gamma k^2}{2} \|\tilde{\beta}\|_2^2$$

$$= \begin{cases} 0 & (\|\tilde{\beta}\|_1 - \theta^\top X\tilde{\beta} \geq 0) \\ \frac{(\|\tilde{\beta}\|_1 - \theta^\top X\tilde{\beta})^2}{2\gamma \|\tilde{\beta}\|_2^2} & (\|\tilde{\beta}\|_1 - \theta^\top X\tilde{\beta} < 0). \end{cases}$$

Because this is stronger than the Fenchel–Young inequality in Eq. (1), the region derived from it and Eq. (8),

$$\left\{ \theta \mid l(\theta; \tilde{\theta}) \leq -\frac{1}{2} \|\theta - y\|_2^2 + \frac{1}{2} \|y\|_2^2 - \min(0, \|\tilde{\beta}\|_1 - \theta^\top X\tilde{\beta}) \right\},$$

is narrower than the region of Gap Safe Sphere. Since this region is a little complex, we propose to use the sphere relaxation.

**General regularized least squares:** Except for Elastic-Net, there are many regularizers that do not satisfy Eq. (7), e.g., squared L1 regularization. In addition, the dual problem of SVM can be seen as the regularized least squares. In those cases, we propose using the upper bound

$$D(\theta) \leq -\frac{1}{2} \|\theta - y\|_2^2 + \frac{1}{2} \|y\|_2^2 + g(\tilde{\beta}) - \theta^\top X\tilde{\beta}.$$

This is based on the Fenchel–Young inequality for $g$ and Eq. (8). Note that the region

$$\{ \theta \mid l(\theta; \tilde{\theta}) \leq -\frac{1}{2} \|\theta - y\|_2^2 + \frac{1}{2} \|y\|_2^2 + g(\tilde{\beta} - \theta^\top X\tilde{\beta}) \}$$

is a sphere in the Gap Safe Sphere region.

**General norm regularized problems:** Here, we extend $f$ to a more general setup, e.g., the logistic loss. Assume that $g$ satisfies Eq. (7). In those cases, we propose using

$$D(\theta) \leq f(X\beta) + \theta^\top X\beta + \inf_{k \geq 0} g(k\tilde{\beta} - \theta^\top X(k\tilde{\beta})),$$

$$= f(X\beta) + \theta^\top X\beta + \begin{cases} 0 & (g(\tilde{\beta}) - \theta^\top X\tilde{\beta} \geq 0) \\ -\infty & (g(\tilde{\beta}) - \theta^\top X\tilde{\beta} < 0). \end{cases}$$

This is based on the Fenchel–Young inequality for $f$ and Eq. (10).