On an improvement of LASSO by scaling

Katsuyuki Hagiwara

Faculty of Education, Mie University,
1577 Kurima-Machiya-cho, Tsu, 514-8507, Japan

Abstract

A sparse modeling is a major topic in machine learning and statistics. LASSO (Least Absolute Shrinkage and Selection Operator) is a popular sparse modeling method while it has been known to yield unexpected large bias especially at a sparse representation. There have been several studies for improving this problem such as the introduction of non-convex regularization terms. The important point is that this bias problem directly affects model selection in applications since a sparse representation cannot be selected by a prediction error based model selection even if it is a good representation. In this article, we considered to improve this problem by introducing a scaling that expands LASSO estimator to compensate excessive shrinkage, thus a large bias in LASSO estimator. We here gave an empirical value for the amount of scaling. There are two advantages of this scaling method as follows. Since the proposed scaling value is calculated by using LASSO estimator, we only need LASSO estimator that is obtained by a fast and stable optimization procedure such as LARS (Least Angle Regression) under LASSO modification or coordinate descent. And, the simplicity of our scaling method enables us to derive SURE (Stein’s Unbiased Risk Estimate) under the modified LASSO estimator with scaling. Our scaling method together with model selection based on SURE is fully empirical and do not need additional hyper-parameters. In a simple numerical example, we verified that our scaling method actually improves LASSO and the SURE based model selection criterion can stably choose an appropriate sparse model.

Keywords:
sparse modeling, LASSO, scaling, SURE

Email address: hagi@edu.mie-u.ac.jp (Katsuyuki Hagiwara)
1. Introduction

A sparse modeling is a major topic in machine learning and statistics. Especially, LASSO (Least Absolute Shrinkage and Selection Operator) is a popular method that has been extensively studied\cite{6, 11, 7, 17, 23, 15, 24}. LASSO is an $\ell_1$ penalized least squares method and has a nature of soft-thresholding that implements thresholding and shrinkage of coefficients; see \cite{4, 5}. These two properties are simultaneously controlled by a single regularization parameter. This causes an excessive shrinkage, thus, a large bias that is directly related to a consistency of model selection by LASSO. This has been pointed out by \cite{12, 7, 15} and it has been proposed several methods for solving this problem\cite{7, 23, 15, 20}. \cite{23} has proposed adaptive LASSO that employs a weighted $\ell_1$ penalty, by which small penalty is assigned to a large coefficient values. \cite{15} has proposed relaxed LASSO to solve a limitation of one parameter control for thresholding and shrinkage by introducing an additional parameter. On the other hand, \cite{7} has proposed SCAD (Smoothly Clipped Absolute Deviation) that employs a non-convex penalty instead of $\ell_1$ penalty. \cite{20} has also introduced a different type of non-convex penalty called MCP (minimax concave penalty). The introduction of non-convex penalty has an effect to suppress a bias at large values of estimators. Since the methods with non-convex penalty have a difficulty in optimization, the solutions to them have been investigated; e.g. \cite{21, 14}. \cite{21} has shown that a gradient descent started from a LASSO solution yields a local minimum of an objective function with a non-convex penalty and it can be a good solution for the objective function. In \cite{14}, local minima in a non-convex penalty method including SCAD and MCP have good quality for true values of coefficients.

In this article, we focus on a model selection problem in applications of a sparse modeling. \cite{22} has shown that LASSO has a consistent model selection property under a certain condition that is, however, known to be somewhat restrictive. On the other hand, under milder conditions than in LASSO, adaptive LASSO, SCAD and MCP have the oracle property that consists of consistency of model selection and asymptotic normality of the estimators of non-zero coefficients\cite{7, 20}. All these results are based on an appropriate setting of the regularization parameter. Therefore, it does not tell us a choice of the regularization parameter in application. Usually, it relies on the cross
validation; e.g. it is commonly implemented in many software packages. We emphasize that a bias problem in LASSO directly affects a choice of model (regularization parameter) under the cross validation. Since a bias is high at a sparse representation in LASSO, a good sparse representation may not be selected by a prediction error based criterion such as cross validation error; see [12]. We need to take into account of this point rather than improvement of estimators. This model selection problem is relaxed in cross validation for adaptive LASSO, SCAD and MCP since a bias problem of LASSO is improved in these methods. However, despite of a good quality of SCAD and MCP estimators as in [21, 14], local minima and optimization problem may yield a fluctuation of estimators among the training sets in cross validation. The impact of this fluctuation on validation error may not be well evaluated. Especially, since these methods need an another hyper-parameter for specifying the shape of penalty term, we need to conduct cross validation for grid search on two hyper-parameters.

In this article, we consider to introduce a scaling of LASSO estimator; i.e. scalar times of LASSO estimator. We here give an appropriate empirical scaling value which actually improves the excessive shrinkage, thus a large bias in LASSO. The empirical scaling value has a simple form with LASSO estimator; i.e. LASSO estimator is plugged in to the scaling value. Therefore, in our method, we just need LASSO estimator that can be obtained by a fast and stable method such as LARS (Least Angle Regression)[6] under LASSO modification or coordinate descent[18, 8]. This is a benefit of our method in comparing with the other methods including non-convex methods. Moreover, a simplicity of our scaling method enables us to derive its analytic model selection criterion that is $C_p$-type criterion based on SURE (Stein’s Unbiased Risk Estimate). For a naive LASSO, SURE has already been derived in [24]. Actually, we apply this result to derive SURE for the LASSO with scaling. However, it is not available for adaptive LASSO, relaxed LASSO and SCAD. Although it is derived for MCP under a specific condition, its effectiveness in applications is not clear; e.g. many software packages that implement MCP employed cross validation. On the other had, our scaling method is closely related to adaptive LASSO and relaxed LASSO. Adaptive LASSO controls biases componentwisely by coefficientwise weights in $\ell_1$ regularizer. The weights are calculated based on the initial estimator such as the least squares estimators. Note that we may need ridge estimators as the initial estimator for stable training in applications. The cost function including the weighted $\ell_1$ regularizer can be simply optimized by a modified
LARS-LASSO[23]. On the other hand, in relaxed LASSO, shrinkage and thresholding parameters are introduced differently and those are simultaneously optimized by an algorithm based on LARS-LASSO. Relaxed LASSO can be viewed as controlling bias independently of threshold. In this point of view, in our scaling method, threshold is achieved by LASSO and amount of shrinkage is controlled by scaling value. Although there have been derived some important asymptotic results for adaptive LASSO and relaxed LASSO, it may be difficult to derive an analytic solution to model selection. On the other hand, as an improvement of adaptive LASSO, multi-step adaptive LASSO has been proposed in [2]; see also [19]. Multi-step adaptive LASSO employ adaptive LASSO at each cycle, in which LASSO estimators are employed as initial estimators in weights. Multi-step adaptive LASSO is similar to our scaling method since both methods employ LASSO estimator in the parameters for improving a bias problem of LASSO. Unfortunately, the method of model selection has not been discussed for multi-step adaptive LASSO. In conclusion, we can say that possibility of deriving SURE is an another benefit of our scaling method.

In section 2, we give a regression framework including LASSO and a definition of risk with its Stein’s formula. In section 3, we introduce a scaling of LASSO estimator. Especially, we give a reasonable empirical scaling value and derive a model selection criterion under the given scaling value. In section 4, we verify our results in section 3 through a simple numerical experiment. It includes comparisons to the other modeling method such as MCP and adaptive LASSO. Section 5 is devoted for conclusions and future works.

2. LASSO with scaling

2.1. Regression problem and LASSO

Let \( x = (x_1, \ldots, x_m) \) and \( y \) be explanatory variables and a response variable, for which we have \( n \) samples : \( \{(x_{i,1}, \ldots, x_{i,m}, y_i) : i = 1, \ldots, n \} \). We define \( x_j = (x_{1,j}, \ldots, x_{n,j})' \in \mathbb{R}^n \) for \( j = 1, \ldots, m \), where ‘ stands for the transpose operator. We define \( X = (x_1, \ldots, x_m) \) and \( y = (y_1, \ldots, y_n)' \). In this article, we assume that \( m \leq n \) holds and \( x_1, \ldots, x_m \) are linearly independent. Therefore, \( X'X \) is not singular here. Let \( \varepsilon_1, \ldots, \varepsilon_n \) be i.i.d. samples from \( N(0, \sigma^2) \); i.e. normal distribution with mean 0 and variance \( \sigma^2 \). Thus, by defining \( \varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)' \), \( \varepsilon \sim N(0_n, \sigma^2 I_n) \), where \( 0_n \) is an \( n \)-dimensional zero vector and \( I_n \) is an \( n \times n \) identity matrix. We assume \( y = \mu + \varepsilon \). We therefore have \( \mu = \mathbb{E}y \), where \( \mathbb{E} \) is the expectation with respect
to the joint probability distribution of \( y \). We consider a regression problem by \( Xb \), where \( b = (b_1, \ldots, b_m) \) is a coefficient vector. Let \( \hat{b} = (\hat{b}_1, \ldots, \hat{b}_m) \) be an estimator of \( b \). LASSO is a method for obtaining coefficient estimators that minimize \( \ell_1 \) regularized cost function defined by

\[
C_\lambda(b) = \|y - Xb\|^2 + \lambda \|b\|_1,
\]

where \( \| \cdot \| \) is the Euclidean norm and \( \|b\|_1 = \sum_{k=1}^{n} |b_j| \). \( \lambda \geq 0 \) is a regularization parameter. The second term of the right hand side of (1) is called \( \ell_1 \) regularizer. Let \( \hat{b}_\lambda = (\hat{b}_{1,\lambda}, \ldots, \hat{b}_{m,\lambda}) \) be a LASSO solution. Since the LASSO is known to yield a sparse representation under an appropriate choice of \( \lambda \), some of elements in \( \hat{b}_\lambda \) are exactly zeros. We denote a LASSO output vector by \( \hat{\mu}_\lambda = (\hat{\mu}_{1,\lambda}, \ldots, \hat{\mu}_{n,\lambda})' \) that is given by \( \hat{\mu}_\lambda = X\hat{b}_\lambda \). We define \( \hat{B}_\lambda = \{i : \hat{b}_{i,\lambda} \neq 0\} \) and \( \hat{k}_\lambda = |\hat{B}_\lambda| \). \( \hat{B}_\lambda \) is called an active set. There are regularization parameter values at which the active set changes. We denote those by \( \lambda_0 > \cdots > \lambda_J = 0 \), in which \( \hat{b}_\lambda = 0_m \) for \( \lambda > \lambda_0 \) under a given \( y \). \( \lambda_j \) is called a transition point.

Let \( X_{\hat{B}_\lambda} \) be an \( n \times \hat{k}_\lambda \) matrix whose column vectors are \( x_j, j \in \hat{B}_\lambda \). We write \( \hat{X}_\lambda = X_{\hat{B}_\lambda} \) for simplicity. Also we define \( \hat{\beta} \) as a \( \hat{k} \)-dimensional vector whose elements are \( \{\hat{b}_k : k \in \hat{B}_\lambda\} \). We write \( \hat{\beta}_\lambda = (\hat{\beta}_{1,\lambda}, \ldots, \hat{\beta}_{\hat{k},\lambda})' \); i.e. \( \hat{\beta}_k \) is a member of \( \{\hat{b}_k : k \in \hat{B}_\lambda\} \) under an appropriate enumeration. Under this definition, we have \( \hat{\mu}_\lambda = \hat{X}_\lambda \hat{\beta}_\lambda \) since \( \hat{b}_{k,\lambda} = 0 \) for \( k \notin \hat{B}_\lambda \). Let \( \hat{S}_\lambda = (\hat{S}_{1,\lambda}, \ldots, \hat{S}_{\hat{k},\lambda})' \) be a sign vector of \( \hat{\beta}_\lambda \); i.e.

\[
\hat{S}_{k,\lambda} = \begin{cases} 
1 & \hat{\beta}_{k,\lambda} > 0 \\
0 & \hat{\beta}_{k,\lambda} = 0 \\
-1 & \hat{\beta}_{k,\lambda} < 0 
\end{cases}
\]

2.2. Some facts on LASSO estimate

By Lemma 1 in [24], the LASSO estimator satisfies that

\[
\hat{\beta}_\lambda = (\hat{X}_\lambda' \hat{X}_\lambda)^{-1} (\hat{X}_\lambda' y - \lambda \hat{S}_\lambda)
\]

if \( \lambda \) is not a transition point. Therefore, we have

\[
\hat{\mu}_\lambda = \hat{H}_\lambda y - \lambda \hat{q}_\lambda,
\]
where $\hat{H}_\lambda = \hat{X}_\lambda (\hat{X}_\lambda' \hat{X}_\lambda)^{-1} \hat{X}_\lambda'$ and $\hat{q}_\lambda = \hat{X}_\lambda (\hat{X}_\lambda' \hat{X}_\lambda)^{-1} \hat{S}_\lambda$. It is easy to check that $\hat{H}_\lambda$ is an idempotent matrix.

We define $\tilde{\beta}_\lambda = (\hat{X}_\lambda' \hat{X}_\lambda)^{-1} \hat{X}_\lambda' y$. This is the least squared estimator under $\hat{X}_\lambda$, thus in a post estimation. Note that this is not a linear estimator of $y$ since $\hat{X}_\lambda$ is already chosen according to $y$. We also define $\tilde{\mu}_\lambda = \hat{X}_\lambda \tilde{\beta}_\lambda$. Obviously, this can be written as $\tilde{\mu}_\lambda = \hat{H}_\lambda y$. Therefore, (4) can be written as

\[
\tilde{\mu}_\lambda = \hat{\mu}_\lambda - \lambda \hat{q}_\lambda
\]  

for a non-transition $\lambda$. We summarize some facts that are derived by (4) and are used in this article.

**Lemma 1.** If $\lambda$ is not a transition point, the following equations hold.

\[
\begin{align*}
\tilde{\mu}' \hat{q}_\lambda &= \|\tilde{\beta}_\lambda\|_1 \\
\|\tilde{\mu}_\lambda\|^2 &= \tilde{\mu}' y - \lambda \hat{q}' y + \lambda^2 \|\hat{q}_\lambda\|^2 \\
\|\tilde{\mu}_\lambda\|^2 &= \tilde{\mu}' y - \lambda \|\tilde{\beta}_\lambda\|_1 \\
\hat{H}_\lambda \tilde{\mu}_\lambda &= \tilde{\mu}_\lambda.
\end{align*}
\]  

*Proof.* In this proof, we drop $\lambda$ from symbols for simplifying the description of terms. By (4), we have

\[
\tilde{\mu}' \hat{q} = \hat{S}' (\hat{X}' \hat{X})^{-1} \hat{X}' (\hat{X}' \hat{X})^{-1} (\hat{X}' y - \lambda \hat{S}) = \hat{S}' \tilde{\beta}.
\]  

We then obtain (6) by the definition of $\hat{S}$.

We define $\tilde{P} = I_n - \hat{H}$. By the definition of $\hat{H}$ and $\tilde{P}$, we have

\[
\hat{q}' \hat{H} y = \hat{q}' y
\]  

and, thus,

\[
\hat{q}' \tilde{P} y = \hat{q}' y - \hat{q}' \hat{H} y = 0.
\]  

Since $\hat{H}$ is an idempotent matrix, we have $\hat{H} \tilde{P} = O_n$, where $O_n$ is an $n \times n$ zero matrix. Thus, by (3), (7) is obtained as

\[
\begin{align*}
\tilde{\mu}' y - \|\tilde{\mu}\|^2 &= \tilde{\mu}' (y - \tilde{\mu}) \\
&= (\hat{H} y - \lambda \hat{q})'(\tilde{P} y + \lambda \hat{q}) \\
&= \lambda \hat{q}' y - \lambda^2 \|\hat{q}\|^2.
\end{align*}
\]  

\[6\]
Moreover, by (11), (4) and (6), we have
\[
\lambda q' y - \lambda^2 \| \hat{q} \|^2 = \lambda q' (\hat{H} y - \lambda q) = \lambda q' \hat{\mu} = \lambda \| \hat{\beta} \|_1. \tag{14}
\]

Finally, by the definition of \( \hat{H} \) and \( \hat{\mu} \), we obtain
\[
\hat{H} \hat{\mu} = \hat{X} (\hat{X}' \hat{X})^{-1} \hat{X}' (\hat{X}' \hat{X})^{-1} (\hat{X}' y - \lambda \hat{S}) = \hat{\mu}. \tag{15}
\]

2.3. Definition of risk and its Stein’s formula

Let \( \hat{\mu} = (\hat{\mu}_1, \ldots, \hat{\mu}_n)' \in \mathbb{R}^n \) be a regression estimate of \( \mu = \mathbb{E}[y] \). A prediction capability of \( \hat{\mu} \) is measured by a risk:
\[
R_n = \frac{1}{n} \mathbb{E} \left[ \| \hat{\mu} - \mu \|^2 \right], \tag{16}
\]
where \( \mathbb{E} \) is the expectation with respect to the joint probability distribution of \( y \). It is easily verified that
\[
R_n = \frac{1}{n} \mathbb{E} \left[ \| \hat{\mu} - y \|^2 \right] - \sigma^2 + DF_n, \tag{17}
\]
where
\[
DF_n = \frac{2}{n} \mathbb{E} [(\hat{\mu} - \mathbb{E}[\hat{\mu}])'(y - \mu)] \tag{18}
\]
that is a covariance between \( \hat{\mu} \) and \( y \). \( DF_n \) is often called the degree of freedom.

Let \( \partial \hat{\mu} / \partial y \) be an \( n \times n \) matrix whose \((i, j)\) entry is \( \partial \hat{\mu}_i / \partial y_j \). We define
\[
\nabla \cdot \hat{\mu} = \text{trace} \left( \frac{\partial \hat{\mu}}{\partial y} \right) = \sum_{i=1}^{n} \frac{\partial \hat{\mu}_i}{\partial y_i} \tag{19}
\]
in which \( \text{trace} \) denotes the trace of a matrix. In [16], it has been shown that
\[
DF_n = \frac{2\sigma^2}{n} \mathbb{E} [\nabla \cdot \hat{\mu}] \tag{20}
\]
holds if $\hat{\mu}_i = \hat{\mu}_i(y) : \mathbb{R}^n \mapsto \mathbb{R}$, $i = 1, \ldots, n$ are almost differentiable in the term of [16] and the expectation in the right hand side exists. $\nabla \cdot \hat{\mu}$ is called a divergence of $\hat{\mu}$. By this result,

$$\hat{R}_n(\sigma^2) = -\sigma^2 \frac{1}{n} \|\hat{\mu} - y\|^2 + \frac{2\sigma^2}{n} \nabla \cdot \hat{\mu}$$  \hspace{1cm} (21)

is an unbiased estimator of a risk $R_n$. $\hat{R}_n(\sigma^2)$ is called SURE (Stein’s Unbiased Risk Estimate). We can then construct a $C_p$-type model selection criterion by replacing $\sigma^2$ with an appropriate estimate $\hat{\sigma}^2$; e.g. [24].

3. LASSO with scaling

3.1. An optimal scaling

We now consider to assign a positive single scaling parameter to LASSO estimator. More precisely, the scaling parameter is denoted by $\alpha > 0$ and the modified LASSO estimator with scaling is given by $\alpha \hat{\beta}_\lambda$, where $\beta_\lambda$ is a vector of non-zero elements of LASSO estimator. The output vector with a single scaling parameter is given by $\hat{\mu}_{\lambda,\alpha} = \alpha \hat{\mu}_\lambda$. Thus, $\hat{\mu}_{\lambda,1}$ is a LASSO output vector. We write $\hat{\mu}_{\lambda,\alpha} = (\hat{\mu}_{\lambda,\alpha,1}, \ldots, \hat{\mu}_{\lambda,\alpha,n})'$, where $\hat{\mu}_{\lambda,\alpha,k} = \alpha \hat{\mu}_{\lambda,k}$.

A risk of LASSO with scaling is

$$R_n(\lambda, \alpha) = \frac{1}{n} \mathbb{E} \left[ \|\hat{\mu}_{\lambda,\alpha} - \mu\|^2 \right].$$ \hspace{1cm} (22)

Especially, $R_n(\lambda, 1)$ is a risk of LASSO. By the previous discussion, it is given by

$$R_n(\lambda, \alpha) = \frac{1}{n} \mathbb{E} \|\hat{\mu}_{\lambda,\alpha} - y\|^2 - \sigma^2 + DF_n(\lambda, \alpha),$$ \hspace{1cm} (23)

where

$$DF_n(\lambda, \alpha) = 2\frac{\sigma^2}{n} \mathbb{E} (\hat{\mu}_{\lambda,\alpha} - \mathbb{E} \hat{\mu}_{\lambda,\alpha})'(y - \mu).$$ \hspace{1cm} (24)

In [24], for LASSO estimate,

$$DF_n(\lambda, 1) = \frac{2\sigma^2}{n} \mathbb{E} \hat{k}_\lambda$$ \hspace{1cm} (25)
has been shown via the above Stein’s formula. By the definition of \( \hat{\mu}_{\lambda, \alpha} \), we thus have

\[
R_n(\lambda, \alpha) = \frac{1}{n} \mathbb{E} \| \alpha \hat{\mu}_\lambda - y \|^2 - \sigma^2 + \frac{2\alpha \sigma^2}{n} \mathbb{E} \hat{k}_\lambda. \tag{26}
\]

Of course, this reduces to a risk of LASSO when \( \alpha = 1 \). By (26), SURE for LASSO is given by

\[
\hat{R}_n(\lambda, \sigma^2) = -\sigma^2 + \frac{1}{n} \| \hat{\mu}_\lambda - y \|^2 + \frac{2\sigma^2}{n} \mathbb{E} \hat{k}_\lambda. \tag{27}
\]

On the other hand, by setting the derivative of (26) with respect to \( \alpha \) to zero, the minimizing scaling value of \( R_n(\lambda, \alpha) \) is given by

\[
\alpha_{\text{opt}} = \frac{\mathbb{E} \hat{\mu}'_\lambda y - \sigma^2 \mathbb{E} \hat{k}_\lambda}{\mathbb{E} \| \hat{\mu}_\lambda \|^2} \tag{28}
\]

if \( \mathbb{E} \| \hat{\mu}_\lambda \|^2 \neq 0 \). If \( \lambda \) is not transition point then we have

\[
\alpha_{\text{opt}} = 1 + \frac{\lambda \mathbb{E} \| \hat{\beta}_\lambda \|_1}{\mathbb{E} \| \hat{\mu}_\lambda \|^2} - \frac{\sigma^2 \mathbb{E} \hat{k}_\lambda}{\mathbb{E} \| \hat{\mu}_\lambda \|^2} \tag{29}
\]

by (8). Through a simple calculation using (26) and (28), we have

\[
R_n(\lambda, 1) - R_n(\lambda, \alpha_{\text{opt}}) = \frac{1}{n} (\alpha_{\text{opt}} - 1)^2 \mathbb{E} \| \hat{\mu}_\lambda \|^2. \tag{30}
\]

Therefore, the optimal scaling value improves naive LASSO at any \( \lambda \). In case of an orthogonal design in a nonparametric regression problem such as wavelet[4, 5], it is shown in [10] that the right hand side of (30) is \( O(n^{-1} \log n) \).

3.2. Data-dependent empirical scaling value

One choice of a scaling value in applications is \( (\hat{\mu}'_\lambda y - \sigma^2 \hat{k}_\lambda)/\| \hat{\mu}_\lambda \|^2 \) that is an empirical estimate of \( \alpha_{\text{opt}} \). In LASSO, \( \hat{\mu}_\lambda = 0_n \) happens to occur when \( \lambda \) is large. Therefore, this scaling value may not be stable. Moreover, the scaling value can be smaller than one depending on the noise variance. Also, it is difficult to handle this estimate since \( \hat{k}_\lambda \) is a dis-continuous function of \( y \). As an another choice, we may have \( \hat{\mu}'_\lambda y/\| \hat{\mu}_\lambda \|^2 \) that minimizes the squared distance between \( y \) and \( \alpha \hat{\mu}_\lambda \); i.e. it approaches LASSO estimator.
to the least squares one. However, again, this may not be stable. Then, for a stable scaling value, we consider

\[ \hat{\alpha} = \frac{\hat{\mu}'_\lambda y + \delta}{\|\hat{\mu}_\lambda\|^2 + \delta}, \]  

(31)

where \( \delta \) is a fixed positive constant. Note that \( \delta \) is not a tuning parameter (hyper-parameter) and is a constant for stabilizing \( \hat{\alpha} \). Therefore, it is set to be a small value, say, \( 10^{-6} \) in applications. By (8), we can write

\[ \hat{\alpha} = 1 + \lambda \|\hat{\beta}_\lambda\|_1 \]  

(32)

for non-transition \( \lambda \). Therefore, \( \hat{\alpha} \geq 1 \) holds; i.e. it really behaves as an expansion parameter. Moreover, \( \hat{\alpha} \approx 1 \) for a small \( \lambda \). This is a nice property since the bias problem in LASSO is serious when \( \lambda \) is large and is not essential when it is small. We have three facts relating to \( \hat{\alpha} \). The first one shows an effect of the introduction of \( \hat{\alpha} \).

**Property 1.** For a non-transition \( \lambda \),

\[ \|y - \hat{\mu}_\lambda\|^2 \leq \|y - \hat{\mu}_{\lambda,\hat{\alpha}}\|^2 \leq \|y - \hat{\mu}_{\lambda,1}\|^2 \]  

(33)

holds.

**Proof.** The first inequality is obvious because \( \hat{\mu}_\lambda \) is the least squares solution under \( \hat{X}_\lambda \); i.e. it is a projection of \( y \) onto a linear subspace determined by column vectors of \( \hat{X}_\lambda \). For simplicity, we define \( m_2 = \|\hat{\mu}_{\lambda,1}\|^2 \) and \( p_1 = \lambda \|\hat{\beta}_\lambda\|_1 \). We then obtain

\[ \|y - \hat{\mu}_{\lambda,\hat{\alpha}}\|^2 \]
\[ = \|y - \hat{\alpha}\hat{\mu}_{\lambda,1}\|^2 \]
\[ = \|y - \hat{\mu}_{\lambda,1} + \hat{\mu}_{\lambda,1} - \hat{\alpha}\hat{\mu}_{\lambda,1}\|^2 \]
\[ = \|y - \hat{\mu}_{\lambda,1}\|^2 + (1 - \hat{\alpha})^2 m_2 + 2(1 - \hat{\alpha})\hat{\mu}'_{\lambda,1}(y - \hat{\mu}_{\lambda,1}) \]
\[ = \|y - \hat{\mu}_{\lambda,1}\|^2 + (1 - \hat{\alpha})^2 m_2 + 2(1 - \hat{\alpha})p_1 \]
\[ = \|y - \hat{\mu}_{\lambda,1}\|^2 + (1 - \hat{\alpha})^2 m_2 - 2(1 - \hat{\alpha})^2(m_2 + \delta) \]
\[ = \|y - \hat{\mu}_{\lambda,1}\|^2 - (1 - \hat{\alpha})^2(m_2 + 2\delta), \]  

(34)

where we used (8) in the fourth line and (32) in the fifth line. \( \square \)
Therefore, the introduction of \( \hat{\alpha} \) surely reduces the residual sum compared to a LASSO estimate. This implies that \( \hat{\alpha} \) moves the LASSO estimator toward the least squares estimator at each \( \lambda \). We here consider

\[
\hat{d}(\lambda) = (1 - \hat{\alpha})^2(m_2 + 2\delta).
\]

(35)

As found in (34), \( \hat{d}(\lambda) \) is the difference between residuals of naive LASSO and LASSO with scaling. Note that this is a function of \( \lambda \) if the training data is given and \( X \) is determined.

**Property 2.** For simplicity, we consider a specific case where \( \delta = 0 \). We assume that \( \|\hat{\beta}_\lambda\|_1 \neq 0 \) holds and \( \lambda \) is a non-transition point. Let \( \rho_{\min} \) and \( \rho_{\max} \) be the minimum and maximum eigenvalues of \( X'X/n \) and assume \( \rho_{\min} > 0 \). Then we have

\[
\frac{\lambda^2}{n\rho_{\max}} \leq \hat{d}(\lambda) \leq \frac{\lambda^2 m^2}{n\rho_{\min}}.
\]

(36)

**Proof.** Since

\[
\hat{d}(\lambda) = \lambda^2 \|\hat{\beta}_\lambda\|_1^2 \left( \|\ell_{\mu,1}\|^2 + 2\delta \right) \|\hat{\mu}\|^2 \|\hat{\beta}_\lambda\|_1^2 = \frac{\lambda^2 \|\hat{\beta}_\lambda\|_1^2}{\|\hat{\mu}\|^2 \|\hat{\beta}_\lambda\|_1^2}
\]

(37)

holds in case of \( \delta = 0 \), we have

\[
\frac{\lambda^2 \|\hat{\beta}_\lambda\|_1^2}{n\rho_{\max} \|\hat{\beta}_\lambda\|_1^2} \leq \hat{d}(\lambda) \leq \frac{\lambda^2 \|\hat{\beta}_\lambda\|_1^2}{n\rho_{\min} \|\hat{\beta}_\lambda\|_1^2}.
\]

(38)

By the equivalence of the norms, this reduces to (36), where we used \( \hat{k}_\lambda \leq m \).

Therefore, the introduction of \( \hat{\alpha} \) improves the degree of fitting to the given data especially when \( \lambda \) is large; i.e. a sparse situation. We next argue on a probabilistic behavior of \( \hat{\alpha} \).

**Property 3.**

\[
\mathbb{E} [\hat{\alpha} - 1] \leq \max \left( \frac{1}{\delta}, \frac{m^2}{\rho_{\min}} \right) \frac{\lambda}{\sqrt{n}}
\]

(39)

holds.
Proof. Since the probability that a fixed $\lambda$ is a transition point is zero as in [24], $\lambda$ is assumed to not be a transition point below. We define an event $E = \{\|\hat{\beta}_\lambda\|_1 \leq \theta_n\}$, where $\theta_n > 0$. $E^C$ denotes the complement of $E$. By (32), we have
\[
E[\hat{\alpha} - 1|E] \leq \frac{1}{\delta} E[\lambda \|\hat{\beta}_\lambda\|_1 | E] \leq \lambda \theta_n / \delta.
\] (40)
We also have
\[
E[\hat{\alpha} - 1|E^C] \leq E \left[ \frac{\lambda \|\hat{\beta}_\lambda\|_1}{n \rho_{\min} \|\hat{\beta}_\lambda\|^2} | E^C \right]
\leq E \left[ \frac{\lambda \kappa}{n \rho_{\min} \|\hat{\beta}_\lambda\|_1} | E^C \right]
\leq \frac{\lambda m^2}{n \rho_{\min} \theta_n}.
\] (41)
Since $E[\hat{\alpha} - 1] = E[\hat{\alpha} - 1|E]P[E] + E[\hat{\alpha} - 1|E^C]P[E^C]$, we have (39) by taking $\theta_n = 1/(2\sqrt{n})$.

We consider the case where $\rho_{\min}$ and $m$ are constants. This is a natural setting of a classical linear regression problem. In this case, by the above result, the expectation of the degree of expansion is bounded above by $O(1/\sqrt{n})$. Therefore, the effect of expansion by $\hat{\alpha}$ is small when $n$ is large and $X$ is fixed. This is also found in the previous result.

3.3. Model selection criterion under empirical scaling

Now, we consider to derive a $C_p$-type model selection criterion for $\hat{\mu}_{\lambda, \hat{\alpha}}$. For this purpose, we derive an unbiased estimate of a risk for $\hat{\mu}_{\lambda, \hat{\alpha}}$. To do this, by (23), we need to calculate the degree of freedom of $\hat{\mu}_{\lambda, \hat{\alpha}}$. We define it by
\[
DF_{sca}^{\alpha}(\lambda) = \frac{2}{n} E \left[ (\hat{\mu}_{\lambda, \hat{\alpha}} - E[\hat{\mu}_{\lambda, \hat{\alpha}}])' (y - \mu) \right].
\] (42)

Theorem 1. We have
\[
DF_{sca}^{\alpha}(\lambda) = \frac{2\sigma^2}{n} E \left[ \hat{d}_1 + \hat{d}_2 \right],
\] (43)
where
\[
\hat{d}_1 = (1 - \hat{\alpha}) \frac{||\hat{\mu}_\lambda||^2 - \delta}{||\hat{\mu}_\lambda||^2 + \delta} \\
\hat{d}_2 = \hat{\alpha} k_\lambda.
\]

(44)

(45)

Proof. We drop \( \lambda \) from expressions for simplicity since we fix \( \lambda \) below. We thus write \( \hat{\beta} = \hat{\beta}_\lambda, \hat{S} = \hat{S}_\lambda, \hat{\mu}_\alpha = \hat{\mu}_{\lambda,\alpha}, \hat{B} = \hat{B}_\lambda \) and \( \hat{k} = \hat{k}_\lambda \).

We can write \( \hat{\mu}_\alpha = \alpha X \hat{B} \hat{\beta} \). Especially, \( \hat{\mu}_1 \) is a LASSO output. For simplicity, we write \( \hat{\mu} = \hat{\mu}_1 \) below. We denote the \( k \)th member of \( \hat{\mu}_\alpha \) by \( \hat{\mu}_{\alpha,k} \).

In [24], it is shown that, for any fixed \( \lambda \), \( \hat{\mu}_{1,k} : \mathbb{R}^n \rightarrow \mathbb{R}, k = 1, \ldots, n \) are almost differentiable. By (31), \( \hat{\alpha} \hat{\mu}_{1,k} : \mathbb{R}^n \rightarrow \mathbb{R} \) is calculated by arithmetic operations of the components of \( y \) and \( \hat{\mu} \). Therefore, \( \hat{\alpha} \hat{\mu}_{1,k} \) is almost differentiable since it essentially requires a coordinate-wise absolutely continuity.

As a result, Stein’s lemma can be applied to \( \hat{\alpha} \hat{\mu}_{\alpha,k} \) and, by (20), we have

\[
DF_{\text{sc}}(\lambda) = \frac{2\sigma^2}{n} \mathbb{E} [\nabla \cdot \hat{\mu}_{\alpha}],
\]

where
\[
\nabla \cdot \hat{\mu}_{\alpha} = \text{trace} \frac{\partial \hat{\mu}_{\alpha}}{\partial y} = \sum_{i=1}^{n} \frac{\partial \hat{\mu}_{\alpha,i}}{\partial y_i}.
\]

(46)

(47)

Since
\[
\sum_{i=1}^{n} \frac{\partial}{\partial y_i} \hat{\mu}_{\alpha,i} = \sum_{i=1}^{n} \hat{\mu}_{1,i} \left( \frac{\partial}{\partial y_i} \hat{\alpha} \right) + \hat{\alpha} \sum_{i=1}^{n} \left( \frac{\partial}{\partial y_i} \hat{\mu}_{1,i} \right),
\]

holds, we have

\[
\nabla \cdot \hat{\mu}_{\alpha} = \hat{\mu}' \left( \frac{\partial \hat{\alpha}}{\partial y} \right) + \hat{\alpha} \nabla \cdot \hat{\mu},
\]

where \( \frac{\partial \hat{\alpha}}{\partial y} \) is an \( n \)-dimensional vector whose \( i \)th entry is \( \frac{\partial \hat{\alpha}}{\partial y_i} \). Since the probability that a fixed \( \lambda \) is a transition point is zero as in [24], \( \lambda \) is assumed to not be a transition point below.

For the second term of (49), it has been shown in [24] that

\[
\frac{\partial \hat{\mu}}{\partial y} = \hat{H}
\]

(50)
by (3) and the local constancy of \( \hat{q} \) under a fixed \( \lambda \). And, we thus have

\[
\nabla \cdot \hat{\mu} = \text{trace} \hat{H} = \hat{k}
\]

(51)

by the idempotence of \( \hat{H} \). Therefore, the second term of (49) is equal to \( \hat{d}_2 \).

We evaluate the first term in below. Since

\[
\frac{\partial}{\partial y_k} \|\hat{\mu}\|^2 = \frac{\partial}{\partial y_k} \sum_{j=1}^n \hat{\mu}_j^2 = 2 \sum_{j=1}^n \hat{\lambda}_j \frac{\partial \hat{\mu}_j}{\partial y_k},
\]

(52)

we have

\[
\frac{\partial \|\hat{\mu}\|^2}{\partial y} = 2 \left( \frac{\partial \hat{\mu}}{\partial y} \right) \hat{\mu} = 2 \hat{H} \hat{\mu} = 2 \hat{\mu}
\]

(53)

by (50) and (9). On the other hand, we have

\[
\frac{\partial \hat{\mu}' y}{\partial y} = \frac{\partial}{\partial y} \left\{ \|\hat{\mu}\|^2 + \lambda \hat{q}' y - \lambda^2 \|\hat{q}\|^2 \right\} = 2 \hat{\mu} + \lambda \hat{q}
\]

(54)

by (53), (7) in Lemma 1 and local constancy of \( \hat{q} \) as in [24].

By (53), (54) and (7) in Lemma 1, we have

\[
\frac{\partial \hat{\alpha}}{\partial y} = \frac{\left( \|\hat{\mu}\|^2 + \delta \right) \frac{\partial \hat{\mu}' y}{\partial y} - (\hat{\mu}' y + \delta) \frac{\partial \|\hat{\mu}\|^2}{\partial y}}{\left( \|\hat{\mu}\|^2 + \delta \right)^2}
\]

\[
= \frac{\left( \|\hat{\mu}\|^2 + \delta \right) (2 \hat{\mu} + \lambda \hat{q}) - 2 (\hat{\mu}' y + \delta) \hat{\mu}}{\left( \|\hat{\mu}\|^2 + \delta \right)^2}
\]

\[
= \frac{\left( \|\hat{\mu}\|^2 + \delta \right) (2 \hat{\mu} + \lambda \hat{q}) - 2 \hat{\alpha} (\|\hat{\mu}\|^2 + \delta) \hat{\mu}}{\left( \|\hat{\mu}\|^2 + \delta \right)^2}
\]

\[
= \frac{1}{\|\hat{\mu}\|^2 + \delta} \{ 2 \hat{\mu} + \lambda \hat{q} - 2 \hat{\alpha} \hat{\mu} \},
\]

(55)
where the third line comes from (31). Therefore, we obtain

\[
\hat{\mu}' \left( \frac{\partial \hat{\alpha}}{\partial y} \right) = \frac{1}{\|\hat{\mu}\|^2 + \delta} \left\{ 2\|\hat{\mu}\|^2 + \lambda \hat{\beta}^T \hat{\beta} - 2\hat{\alpha} \|\hat{\mu}\|^2 \right\} = \frac{2}{\|\hat{\mu}\|^2 + \delta} (1 - \hat{\alpha}) \|\hat{\mu}\|^2 + \frac{\lambda \|\hat{\beta}\|_1}{\|\hat{\mu}\|^2 + \delta}
\]

\[
= \frac{2}{\|\hat{\mu}\|^2 + \delta} (1 - \hat{\alpha}) \|\hat{\mu}\|^2 + \frac{\hat{\mu}' y + \delta - \|\hat{\mu}\|^2}{\|\hat{\mu}\|^2 + \delta}
\]

\[
= \frac{2}{\|\hat{\mu}\|^2 + \delta} (1 - \hat{\alpha}) \|\hat{\mu}\|^2 - (1 - \hat{\alpha})
\]

\[
= (1 - \hat{\alpha}) \|\hat{\mu}\|^2 - \delta
\]

(56)

where we used (31) and (6), (8).

We have two remarks on this theorem.

- Our discussion is always applicable when \(XX^T\) is not singular.
- \(\mathbb{E}[\hat{d}_1] \leq O(1/\sqrt{n})\) by Lemma 3 since \(|\hat{d}_1| \leq \hat{\alpha} - 1\).

By this theorem, the risk for \(\hat{\mu}_{\lambda,\hat{\alpha}}\) is given by

\[
R_n^{\text{ sca}}(\lambda) = \frac{1}{n} \mathbb{E} \left[ \|\mu - \hat{\mu}_{\lambda,\hat{\alpha}}\|^2 \right]
\]

\[
= -\sigma^2 + \frac{1}{n} \mathbb{E} \left[ \|y - \hat{\mu}_{\lambda,\hat{\alpha}}\|^2 \right] + DF_n^{\text{ sca}}(\lambda).
\]

(57)

Therefore, SURE for LASSO with scaling is given by

\[
\hat{R}_n^{\text{ sca}}(\lambda, \sigma^2) = -\sigma^2 + \frac{1}{n} \|y - \hat{\mu}_{\lambda,\hat{\alpha}}\|^2 + \frac{2\sigma^2}{n} \left( \hat{d}_1 + \hat{d}_2 \right),
\]

(58)

where \(\hat{d}_1\) and \(\hat{d}_2\) are defined by (44) and (45) respectively.
3.4. Estimate of noise variance

To compute a $C_p$-type model selection criterion based on SURE, we need an appropriate estimate of $\sigma^2$. For estimating the noise variance in a regression problem, [3] has recommended to apply

$$\hat{\sigma}_{CE}^2 = \frac{y'(I_n - H_{\gamma})^2 y}{\text{trace}[(I_n - H_{\gamma})^2]},$$

(59)

where $H_{\gamma} = X(X'X + \gamma I_n)^{-1}X'$ with $\gamma > 0$. $H_{\gamma}$ can be viewed as the hat matrix in a ridge regression with a ridge parameter $\gamma > 0$ or, equivalently, an $\ell_2$ regularization with a regularization parameter $\gamma$. In general, the $\ell_2$ regularization is introduced for better generalization and stabilization. We need to carefully select the parameter value for the former reason. However, since the purpose to introduce $\gamma$ here is to stabilize an estimate of the noise variance. Therefore, we just set $\gamma$ to a small value, say, $10^{-6}$ in applications. Especially, this is effective when $m$ is large; i.e. when a colinearity problem arises under a full model.

4. Numerical examples

In this section, through a simple numerical example, we verify our result on SURE for LASSO with scaling and compare our method with naive LASSO, MCP and Adaptive LASSO. We refer to Adaptive LASSO as A-LASSO and LASSO with scaling $\hat{\alpha}$ as LASSO-S.

4.1. Setting of experiments

For $u \in \mathbb{R}$, we define $g_\tau(u, \xi) = \exp\{(u - \xi)^2/(2\tau)\}$, where $\xi \in \mathbb{R}$ and $\tau > 0$. Let $u_i$, $i = 1, \ldots, n$ be equidistant points in $[-5, 5]$. Let $\{\xi_1, \ldots, \xi_m\}$ be a subset of $\{u_1, \ldots, u_n\}$, where $m \leq n$. We take $\xi_j = u_{(n/m)j}$, $j = 1, \ldots, m$ by assuming $n/m$ is an integer. We define $n \times m$ matrix $X_1$ whose $(i, j)$ entry is $g_\tau(u_i, \xi_j)$; i.e. the $j$th column vector of $X_1$ is an output vector of $g_\tau(\cdot, \xi_j)$. Let $X_2$ be a normalized version of $X_1$; i.e. the mean and squared norm of each column vector of $X_2$ are equal to zero and $n$ respectively. By taking account of the intercept, we construct a design matrix by $X = (1_n, X_2)$. Therefore, we consider a curve fitting problem using a linear combination of $m$ Gaussian basis functions whose centers are input data points that are appropriately chosen. We generate $y_i$ by $y_i = \sum_{k=1}^m \beta_{k}^* g_\tau(u_i, \xi_k) + \varepsilon_i$, where $\varepsilon_i \sim N(0, \sigma^2)$. We define $K^* = \{k|\beta_{k}^* \neq 0\}$ and consider the case where $|K^*| \ll m$. This corresponds to the case that there exists an exact sparse representation; i.e. there is a small true representation.
4.2. Verification of risk estimate

In the first numerical experiment, we verify our theoretical result of SURE for LASSO-S. We here refer to \( \hat{R}_n(\lambda, \hat{\sigma}^2_{CE}) \) in (27) and \( \hat{R}^\text{scn}(\lambda, \hat{\sigma}^2_{CE}) \) in (58) as SUREs of LASSO and LASSO-S respectively; i.e. the noise variance is replaced with \( \hat{\sigma}^2_{CE} \) defined in (59). These are fully empirical and, thus, can be applied as model selection criteria.

We set \( n = 100, m = 50, \sigma^2 = 1, \tau = 0.1, K^* = \{5, 18, 31, 45\} \) and \( (\beta_5^*, \beta_{18}^*, \beta_{31}^*, \beta_{45}^*) = (1, -2, 2, -1) \); i.e. \( \xi_j \)'s of non-zero coefficients are almost equally positioned. We also set \( \delta = 1/n \) for LASSO-S and \( \gamma = 10^{-6} \) in calculating \( \hat{\sigma}^2_{CE} \). We here consider two cases of \( \tau = 0.1 \) and \( \tau = 0.4 \). In both cases, some Gaussian functions that are close to each other are relatively correlated. However, 4 Gaussian functions with non-zero coefficients (components of a target function) are nearly orthogonal in the former case while those are still correlated in the latter case. This condition of correlation among components in a target function affects the consistency of model selection of LASSO, A-LASSO and MCP.

We here employ LARS-LASSO for calculating LASSO path[6] and use “lars” package[6] in R. Since the regularization parameter corresponds to the number of un-removed coefficients, we here observe the relationship between the number of un-removed coefficients and risk. Since we know the true representation, we can calculate the actual risk by the mean squared error between the true output and estimated output. We repeat this procedure for 1000 times and calculate averages of actual risks and SUREs.

The averages of actual risks and SUREs of LASSO and LASSO-S are depicted in Fig.1. The horizontal axis is an average of the number of non-zero coefficients (members in active set) at each step in LARS-LASSO. Note that, at a fixed step of LARS-LASSO, the number of non-zero coefficients may be different for 1000 trials. Therefore, we take an average of those; i.e. the horizontal axis corresponds to the number of LARS-LASSO steps while we show the number of averages of non-zero coefficients at the steps in the horizontal axis. In Fig.1, we depict the results at some specific steps (not the results at all steps) for the clarity of graphs. We have some remarks on these results.

- SURE is well consistent with the actual risk for both of LASSO and LASSO-S. Especially, the consistency for LASSO-S verifies Theorem 1.
- When the number of non-zero coefficients is small (\( \lambda \) is large), LASSO-S shows a lower risk compared to LASSO. This is notably for \( \tau = 0.1; \)
i.e. components of a target function are nearly orthogonal.

- The number of non-zero coefficients at which an averaged risk is minimized is smaller for LASSO-S than LASSO. This is also notable for \( \tau = 0.1 \).

As a result, we can expect that \( \hat{R}^{\text{scale}}_n(\lambda, \hat{\sigma}_{\text{CE}}^2) \) can be a good selector of \( \lambda \) in applications; i.e. it can choose a sufficiently sparse model with low risk.

4.3. Comparison to the other methods

We here compare LASSO, LASSO-S, MCP and A-LASSO in the previous setting of experiment although we test the cases of \( n = 100 \) and \( n = 400 \). We use “glmnet” package[9] for LASSO, LASSO-S, A-LASSO and “ncvreg” package[1] for MCP in R. We conduct simulations of model selection in which the number of simulations is \( S = 100 \). Basically, in all methods, the candidate values of the regularization parameter is 20 points in \([0.01, 0.5]\) with log-scale. In LASSO and LASSO-S, we employ SUREs with \( \hat{\sigma}_{\text{CE}}^2 \) for model selection. In A-LASSO, the weight for the penalty term is set to the reciprocal of the absolute value of the ridge estimator. This is a substitute of the least squares estimator to avoid a collinearity problem. The ridge parameter in doing this is selected by 10-fold cross validation in 10 points in \([0.01, 10]\) with log-scale. By using this initial estimator, the regularization parameter of A-LASSO and \( \gamma \)-parameter (exponent of weights) are selected by a grid search of 10-fold cross validation in which the candidate values for \( \gamma \)-parameter are \{0.5, 1.0, 2.0\}. For MCP, the regularization parameter and \( \gamma \)-parameter are selected by a grid search of 10-fold cross validation, in which the candidate values of \( \gamma \)-parameter are \{2.5, 3.0, 3.5, 4.0\}. In MCP, the choice of \( \gamma \)-parameter seems to largely affect the generalization performance. At each simulation, we calculate the number of non-zero coefficients and actual risk of a selected model. The boxplots of risk and the number of non-zero coefficients of a selected model is depicted in Fig.2 and Fig.3 for \( \tau = 0.1 \) and Fig.4 and Fig.5 for \( \tau = 0.4 \).

In Fig.2 and Fig.3, we can see that LASSO-S tends to select a sparse model with lower risk in comparing with LASSO. Especially, selection of a sparse representation of LASSO-S is notable. This shows that our scaling method surely contributes to improve model selection property even though it is a simple modification of LASSO. Therefore, the introduction of scaling really solves the bias problem of LASSO. LASSO-S is also comparable or
Figure 1: Averages of actual risks and SUREs for LASSO and LASSO-S.
Figure 2: Risk of selected model ($\tau = 0.1$).

(a) $n = 100$

(b) $n = 400$
Figure 3: The number of non-zero coefficients of selected model ($\tau = 0.1$).

(a) $n = 100$

(b) $n = 400$
Figure 4: Risk of selected model (τ = 0.4).
Figure 5: The number of non-zero coefficients of selected model ($\tau = 0.4$).
superior to A-LASSO in terms of both of sparseness and risk even though we choose the hyper-parameters in A-LASSO by cross validation. MCP shows the best performance in sparseness and risk. This is notable when \( n = 400 \), relatively large sample case. However, when \( n = 100 \), risk of MCP tends to be larger than the other methods in some data.

On the other hand, as mentioned above, Fig.4 and Fig.5 show results when components in a target function are relatively correlated. In this case, we can see that MCP shows a worse total performance compared to the other methods even when \( n = 400 \). Contrastly, LASSO-S shows the best performance while LASSO also shows a good performance. These results tell us that LASSO-S bring us a stable improvement of LASSO regardless the number of samples and condition on a target function. Additionally, both of optimization and model choice of LASSO-S is very simple and fast.

5. Conclusions and future works

LASSO is known to be suffered from a bias problem that is caused by excessive shrinkage. In this article, we considered to improve it by a simple scaling method. We gave an appropriate empirical scaling value that expands LASSO estimator and actually moves LASSO estimator close to the least squares estimator of the post estimation. This is shown to be especially effective when the regularization parameter is large; i.e. a sparse representation. Since it can be calculated based of LASSO estimator, we just run a fast and stable LASSO optimization procedure such as LARS-LASSO or coordinate descent. We also derived SURE under the modified LASSO with scaling. This analytic solution for model selection is also a benefit of the proposed scaling method. As a result, we gave a fully empirical sparse modeling procedure by a scaling method. In a simple numerical example, we verified that the proposed scaling method actually fixes the problem in LASSO and has a stability of model selection compared to MCP and adaptive LASSO. As a future works, we need more application results of our scaling method. Although we considered to assign a single scaling value for all coefficients in this article, the assignment of coefficient-wise scaling values is expected to improve a prediction performance. This extension of our scaling method is also a part of future works.
Acknowledgements

This work was supported in part by Japan Society for the Promotion of Science (JSPS) KAKENHI Grant Number 18K11433.

References

[1] Breheny, P. and Huang, J., 2011. Coordinate descent algorithms for nonconvex penalized regression, with applications to biological feature selection. Ann. Appl. Statist., 5, 232-253.

[2] Bühlmann, P., Meier, L. 2008. Discussion: One-Step Sparse Estimates in Nonconcave Penalized Likelihood Models, Ann. Stat. 2008, 36, 1534-1541.

[3] Carter, C.K., Eagleson, G.K., 1992. A comparison of variance estimators in nonparametric regression. J. R. Statist. Soc. B, 54, 773-780.

[4] Donoho, D.L., Johnstone, I.M., 1994. Ideal spatial adaptation via wavelet shrinkage. Biometrika, 81, 425-455.

[5] Donoho, D.L., Johnstone, I.M., 1995. Adapting to unknown smoothness via wavelet shrinkage. J. Amer. Statist. Assoc., 90, 1200-1224.

[6] Efron, B., Hastie, T., Johnstone, I., Tibshirani, R., 2004. Least angle regression. Ann. Statist. 32, 407-499.

[7] Fan, J., Li, R., 2001. Variable selection via nonconcave penalized likelihood and its oracle properties. J. Amer. Statist. Assoc. 96, 1348-1360.

[8] Friedman, J., Hastie, T., Hofling, H., Tibshirani, R., 2007. Pathwise coordinate optimization. Ann. Appl. Statist., 1, 302-332.

[9] Friedman, J., Hastie, T., Tibshirani, R., 2010. Regularization Paths for Generalized Linear Models via Coordinate Descent. Journal of Statistical Software, 33, 1-22.

[10] Hagiwara, K., 2016. On scaling of soft-thresholding estimator. Neurocomputing, 194, 360-371.

[11] Knight, K., Fu, W., 2000. Asymptotics for Lasso-Type Estimators. Ann. Stat. 28, 1356-1378.
[12] Leng, C.L., Lin, Y., Wahba, G., 2006. A Note on the lasso and related procedures in model selection. Statistica Sinica, 16, 1273-1284.

[13] Liu, H., Yao, T., Li, R., 2016. Global solutions to folded concave penalized nonconvex learning. Ann. Stat., 44, 629-659.

[14] Loh, P.L., Wainwright, M.J., 2015. Regularized M-estimators with nonconvexity: Statistical and algorithmic theory for local optima. Journal of Machine Learning Research, 16, 559-616.

[15] Meinshausen, N., 2007. Relaxed Lasso. Computational statistics & data analysis, 52, 374-393.

[16] Stein, C., 1981. Estimation of the mean of a multivariate normal distribution. Ann. Stat. 9, 1135-1151.

[17] Tibshirani, R., 1996. Regression shrinkage and selection via the lasso. J. R. Statist. Soc. Ser. B. 58, 267-288.

[18] Wu, T.T, Lange, K., 2008. Coordinate descent algorithms for LASSO penalized regression. Ann. Appl. Stat. 2, 224-244.

[19] Xiao, N., Xu, Q.S., 2015. Multi-step adaptive elastic-net: reducing false positives in high-dimensional variable selection, Journal of Statistical Computation and Simulation, 85, 3755-3765.

[20] Zhang, C.H., 2010. Nearly unbiased variable selection under minimax concave penalty. Ann. Stat., 38, 894-942.

[21] Zhang, C.H., Zhang, T., 2012. A general theory of concave regularization for high-dimensional sparse estimation problems. Statistical Science, 27, 576-593.

[22] Zhao, P., Yu, B., 2006. On model selection consistency of LASSO. Journal of Machine Learning Research, 7, 2541-2563.

[23] Zou, H., 2006. The adaptive lasso and its oracle properties. J. Amer. Statist. Assoc. 101, 1418-1492.

[24] Zou, H., Hastie, T., Tibshirani, R., 2007. On the degree of freedom of the LASSO. Ann. Statist. 35, 2173-2192.