Bridging between soft and hard thresholding by scaling

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Abstract—Thresholding methods are simple and typical examples of sparse modeling. Also they are successfully applied in wavelet denoising in statistical signal processing. In this article, we developed and analyzed a thresholding method in which soft thresholding estimators are independently expanded by empirical scaling values. The scaling values have a common hyper-parameter that is an order of expansion of an ideal scaling value that achieves hard thresholding. We simply call this estimator a scaled soft thresholding estimator. The scaled scaling value that achieves hard thresholding. We simply call this estimator a scaled soft thresholding estimator. The scaled soft thresholding is a general method that includes the soft thresholding and non-negative garrote as special cases and gives an another derivation of adaptive LASSO. We then derived the degree of freedom of the scaled soft thresholding by means of the Stein’s unbiased risk estimate and found that it is decomposed into the degree of freedom of soft thresholding and the reminder connecting to hard thresholding. In this meaning, the scaled soft thresholding gives a natural bridge between soft and hard thresholding methods. Since the degree of freedom represents the degree of over-fitting, this result implies that there are two sources of over-fitting in the scaled soft thresholding. The first source originated from soft thresholding is determined by the number of un-removed coefficients and is a natural measure of the degree of over-fitting. We analyzed the second source in a particular case of the scaled soft thresholding by referring a known result for hard thresholding. We then found that, in a sparse, large sample and non-parametric setting, the second source is largely determined by coefficient estimates whose true values are zeros and has an influence on over-fitting when threshold levels are around noise levels in those coefficient estimates. In a simple numerical example, these theoretical implications have well explained the behavior of the degree of freedom. Moreover, based on the results here and some known facts, we explained the behaviors of risks of soft, hard and scaled soft thresholding methods. These insights together with the result of a simple numerical example showed the advantage of the bridge methods, especially the scaled soft thresholding, in applications.

Index Terms—bridge thresholding method, non-negative garrote, soft thresholding, hard thresholding, SURE

I. INTRODUCTION

Regularization methods are important tools in machine learning. Especially, there are many regularization methods for sparse modeling such as LASSO (Least Absolute Shrinkage and Selection Operator) [13], MCP (Minimax Concave Penalty) [19], AL (adaptive LASSO) [20], NG (Non-negative Garrote) [1], [15]; e.g. see also [7], [20]. LASSO is an $\ell_1$ penalized least squares method and has a nature of soft-thresholding that implements thresholding and shrinkage of coefficients; e.g. [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 weakness of consistency of model selection by LASSO. This fact has been pointed out by [7], [10] and several methods have been proposed for solving this problem as seen in MCP and the others [7], [20]. In these investigations, they discussed the selection consistency under an appropriate choice of regularization parameter. However, we need to choose it based on data in applications. Cross validation is often employed to do this while there are a few analytic approaches for model selection. For LASSO, [3], [14] have derived SURE (Stein’s Unbiased Risk Estimate) to choose a regularization parameter. This is possible because the solution to LASSO is tractable while it is not explicit. Unfortunately, in general, analytic investigation of a model selection problem is difficult for the improvements of LASSO due to the complex and implicit solution.

Many regularization methods for sparse modeling can be explicitly represented as thresholding methods in case of orthogonal regression problems. For example, it is well known that LASSO reduces to ST (Soft Thresholding). Also, MCP and NG have simple closed forms of coefficient estimates in orthogonal design [8], [9], [20]; e.g. FT (Firm Thresholding) in [9] is a special case of MCP. Actually, SURE for ST is well known; e.g. [6]. Also, SURE has been derived for FT in [19] and NG thresholding in [8]. The thresholding methods are important not only in the analysis of sparse modeling but also in applications. Especially, a non-parametric version of orthogonal regression is important in statistical signal processing as seen in the success of wavelet denoising [4], [5]. Due to a possibility of analytic treatment and a significance in applications, we consider thresholding methods of non-parametric orthogonal regression problems in this article.

The above improvements of LASSO are intended to reduce biases of non-zero coefficient estimates in LASSO. Therefore, the estimates move to the least squares ones in these improvements. In this meaning, the terminal of them is an $\ell_0$ regularization method and some of them can be bridges for linking $\ell_1$ regularizer to $\ell_0$ one. For example, MCP and AL

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A. Non-parametric orthogonal regression

Let \((x_i, y_i), i = 1, \ldots, n\) be samples in which \(x_i = (x_{i1}, \ldots, x_{in})\). Let \(X\) be an \(n \times n\) design matrix whose \((i, j)\) element is \(x_{ij}\). We define \(y = (y_1, \ldots, y_n)^T\), where \(^T\) denotes the transpose of a matrix. We here consider a regression problem by \(X\beta\) of \(y\), where \(\beta = (\beta_1, \ldots, \beta_n)^T\) is a coefficient vector. This is a non-parametric regression problem.

We especially assume that the orthogonality of design; i.e. \(X^TX = nI_n\), where \(I_n\) is an \(n \times n\) identity matrix. A typical example of this problem is discrete wavelet transform in signal processing. For example, in time series applications, we set \(x_{i,j} = g_j(t_i)\), where \(g_j\) is a univariate wavelet function and \(t_i\) is the \(i\)th sampling time.

We assume that \(y\) is generated by the rule:

\[ y = X\beta + \varepsilon, \]

where \(\beta = (\beta_1, \ldots, \beta_n)^T\) and \(\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)^T\). We also assume i.i.d Gaussian additive noise; i.e. \(\varepsilon \sim N(0_n, \sigma^2I_n)\), where \(0_n\) is an \(n\)-dimensional zero vector and \(\sigma^2\) is a noise variance. Here, \(\beta\) is a true coefficient vector. We define \(K^* = \{k : \beta_k \neq 0\}\) and \(k^* = |K^*|\) that is the number of members of \(K^*\). In a sparse setting, we may assume that \(k^* \ll n\). It is easy to see that

\[ \hat{\beta} = \frac{1}{n}X^Ty \]

is the least squares estimate and \(y = X\hat{\beta}\); i.e. it is a transformation of \(y\). We have \(\hat{\beta} \sim N(\beta, \sigma^2I_n/n)\) under the assumption on \(\varepsilon\). Therefore, \(\hat{\beta}_1, \ldots, \hat{\beta}_n\) are mutually independent and \(\hat{\beta}_k \sim N(\beta_k, \tau_n^2/n)\), where we define \(\tau_n = \sigma/\sqrt{n}\).

B. Risk and degree of freedom

Let \(\hat{\beta} = (\hat{\beta}_1, \ldots, \hat{\beta}_n)^T\) be an estimate that is calculated by \(\hat{b}\); i.e. \(\hat{\beta} = \hat{\beta}(\hat{b})\) that is a modification of the least squares estimate. We define \(\hat{\mu} = X\hat{\beta}\) and \(\mu = X\beta\). Let \(E_y\) denotes the expectation with respect to the joint probability distribution of \(y\). We define the risk by

\[ R_n = \frac{1}{n}E_y\|\hat{\mu} - \mu\|^2 \]

By defining

\[ D_n = E_y(\hat{\mu} - E_y\hat{\mu})^T(y - \mu), \]

it is easy to see that

\[ R_n = \frac{1}{n}E_y\|y - \hat{\mu}\|^2 - \sigma^2 + \frac{2}{n}D_n \]

holds, where we used \(E_yy = \mu\) and \(y \sim N(\mu, \sigma^2I_n)\). \(D_n\) is the covariance between \(\hat{\mu}\) and \(y\). Since \(\varepsilon = y - \mu\), the DOF can be regarded as a measure of over-fitting (to noise). \(D_n\) is called the degree of freedom (DOF). It is also called the optimism in \([13]\). From the above viewpoint, it can be also regarded as the degree of over-fitting (DOOF). If the model complexity increases then DOOF is high and, thus, the DOF is high. As a typical example, the number of variables is a measure of the model complexity. Actually, as well known in case of the least squares estimation, the DOF is the sum of the variances of estimators and in proportion to the number of variables.

In the expectation, we can replace \(y\) with \(\hat{b}\) by the change of variables and further have

\[ D_n = nE_{\hat{b}}(\hat{\beta} - E\hat{\beta})^T(\hat{b} - b) = nE_{\hat{b}}\hat{\beta}^T(\hat{b} - b) \]

since \(E_{\hat{b}}\hat{b} = b\), where \(E_{\hat{b}}\) is the expectation with respect to the joint distribution of \(\hat{b}\). We further assume that \(\beta_k\) is calculated only by \(\hat{b}_k\); i.e. \(\beta_k = \beta_k(\hat{b}_k)\) and the others are not included in calculating \(\beta_k\). The estimates considered in this article satisfy this condition. In this case, we can write

\[ D_n = n \sum_{k=1}^{n} E_{\hat{b}_k} \beta_k(\hat{b}_k - b_k), \]

where \(E_{\hat{b}_k}\) is the expectation with respect to the marginal distribution of \(\hat{b}_k\).

In case of the least squares method, as well known, the DOF corresponds to the variance of the estimator; i.e. in case of \(\beta_k(\hat{b}_k) = \hat{b}_k\). However, this does not hold in general.

Since \(\hat{b}_k \sim N(b_k, \sigma^2/n)\), the Stein’s lemma for this case states that

\[ E_{\hat{b}_k} \beta_k(\hat{b}_k - b_k) = E_{\hat{b}_k} \frac{\partial \beta_k}{\partial b_k} \]
holds if \( \hat{\beta}_k = \hat{\beta}_k(\hat{b}_k) \) is absolutely continuous as a function of \( \hat{b}_k \) and, of course, the right hand side exists. Therefore, we have

\[
D_n = \sigma^2 \sum_{k=1}^{n} \mathbb{E}_b \left[ \frac{\partial \hat{\beta}_k}{\partial \hat{b}_k} \right] = \sigma^2 \mathbb{E}_b \sum_{k=1}^{n} \frac{\partial \hat{b}_k}{\partial \hat{b}_k}.
\]

(9)

This tells us that the DOF is determined by the degree of variation of \( \hat{\beta}_k \) with respect to \( \hat{b}_k \). This is natural since the DOF is the covariance between a modified estimator and the least squares estimator; i.e., \( \hat{\beta}(\hat{b}) \) and \( \hat{b} \). The covariance can be large when the variation of \( \hat{\beta}_k \) is large. For example, if we simply consider \( \hat{\beta}_k = \gamma \hat{b}_k \) with \( \gamma > 1 \) then the DOF is proportional to \( \gamma \) while such an estimation cannot show a good performance. If the degree of variation changes with \( \hat{b}_k \) then the DOF is large when a large variation occurs around the point at which the probability density is high.

The unbiased estimate of \( R_n \) with the representation of \( \mathcal{R} \) is called Stein’s Unbiased Risk Estimate (SURE). We simply use \( \mathbb{E} \) for \( \mathbb{E}_b \) and \( \mathbb{E}_k \) for \( \mathbb{E}_{\hat{b}_k} \) below.

III. SOME EXISTING THRESHOLDING METHODS AND THEIR SUREs

We here list some existing thresholding methods that are induced by regularization method. Those include HT, ST, NG and FT. All of these are explicitly represented as a function of \( \hat{b}_k \) for each \( k \). For a set \( E \), we denote the complement of \( E \) by \( \overline{E} \). We define

\[
I_E(u) = \begin{cases} 
1 & u \in E \\
0 & u \notin E 
\end{cases}
\]

(10)

for \( u \in \mathbb{R} \) and \( E \subseteq \mathbb{R} \). We define

\[
I_\lambda(u) = 1 - I_{(-\lambda, \lambda)}(u)
\]

(11)

which is an index function on \((-\lambda, \lambda)\). We also define \((u, 0)_+ = \max(u, 0)\).

A. Hard thresholding (HT)

We define a hard thresholding function by

\[
H_\lambda(u) = uI_\lambda(u)
\]

(12)

where \( \lambda > 0 \) is a parameter that is a threshold level. The HT estimator is obtained by

\[
\hat{\beta}_k^{\text{HT}} = H_\lambda(\hat{b}_k)
\]

(13)

This corresponds to an \( \ell_0 \) regularized estimate from a view point of regularization. We define

\[
\hat{K}_\lambda = \{ k : |\hat{b}_k| \geq \lambda \}
\]

(14)

and \( \hat{b}_\lambda = |\hat{K}_\lambda| \). Note that \( \hat{K}_\lambda \) is often called an active set or a support. Since \( H_\lambda \) is not continuous, we cannot apply the Stein’s lemma. As shown in \[18\] and also in the later section, it is possible to evaluate the DOF of HT by using different ways. However, we find that it is useless in applications since we need information on a true representation for constructing SURE. Instead of applying SURE, there are some proposals of determining an optimal threshold level of HT; e.g. \[4\], \[5\].

B. Soft thresholding (ST)

Let sign be a sign function. We define a soft thresholding function by

\[
S_\lambda(u) = \begin{cases} 
\text{sign}(u)\lambda & |u| \geq \lambda \\
0 & |u| < \lambda 
\end{cases}
\]

(15)

where \( \lambda > 0 \) is a parameter for simultaneously determining both of threshold level and amount of shrinkage. For that of HT for the same value of \( \lambda \). The estimates in the active set are shrunk towards zero in ST by \( \lambda \). We denote the DOF of ST by \( D_n^{\text{ST}}(\lambda) \). Since we have

\[
\frac{\partial S_\lambda}{\partial \hat{b}_k} = I_{\lambda}(\hat{b}_k),
\]

(16)

we obtain

\[
D_n^{\text{ST}}(\lambda) = \sigma^2 \sum_{k=1}^{n} I_{\{ \hat{b}_k \}} = \sigma^2 \sum_{k=1}^{n} I_{\{ \hat{b}_k \}}
\]

(17)

by the Stein’s lemma. This result is typically useful in applications since we have SURE :

\[
\mathcal{R}_n = \frac{1}{n} \| \mathbf{y} - \mathbf{X} \hat{\beta}^{\text{ST}} \|^2 - \sigma^2 + \frac{2\sigma^2}{n} I_{\lambda}(\hat{b}_k)
\]

(18)

where \( \hat{\beta}^{\text{ST}} = (\hat{\beta}_1^{\text{ST}}, \ldots, \hat{\beta}_n^{\text{ST}})' \). This can be \( C_\alpha \)-type model selection criterion \[11\] when we can obtain an appropriate estimate of \( \sigma^2 \) in applications; e.g. median absolute deviation (MAD) estimate for the first detail coefficients in wavelet decomposition \[4\], \[5\].

C. Non-negative garrote (NG)

NG is a regularization method \[11\], \[15\], \[20\] and can be explicitly solved in an orthogonal case \[11\], \[8\], which has been given by

\[
\hat{\beta}_k^{\text{NG}} = (1 - \lambda^2/|\hat{b}_k|^2) \hat{b}_k.
\]

(19)

It is easily understood that NG can relax a bias problem of ST at large absolute value of coefficient estimates. If we define

\[
\hat{\alpha}_k = \begin{cases} 
1 + \lambda/|\hat{b}_k| & |\hat{b}_k| \geq \lambda \\
2 & |\hat{b}_k| < \lambda 
\end{cases}
\]

(20)

then it is easy to see that the NG estimate is written as

\[
\hat{\beta}_k^{\text{NG}} = \hat{\alpha}_k S_\lambda(\hat{b}_k)
\]

(21)

In the definition of \( \hat{\alpha}_k \), the value for \( |\hat{b}_k| < \lambda \) is not important since \( S_\lambda(\hat{b}_k) = 0 \) in this area. The definition guarantees the continuity of \( \hat{\alpha}_k \) formally. This is a scaled ST estimate with a
scaling value $\hat{\alpha}_k$ \(^{(17)}\). We denote the DOF for NG by $D_n^{NG}(\lambda)$. Since we have

$$\frac{\partial D_n^{NG}(\lambda)}{\partial \hat{b}_k} = (1 + \lambda^2 / |\hat{b}_k|^2) I_\lambda(\hat{b}_k),$$

we obtain

$$D_n^{NG}(\lambda) = \sigma^2 E \hat{K}_\lambda + \sigma^2 E \sum_{k \in K_\lambda} \frac{\lambda^2}{|\hat{b}_k|^2}$$

by the Stein’s lemma; e.g. see also \(^{(8)}\). Note that the first term of $D_n^{NG}(\lambda)$ is the DOF of ST.

### D. Firm thresholding (FT)

MCP \(^{(19)}\) is a regularization method with non-convex penalty, by which a bias problem of LASSO is known to be relaxed. In the orthogonal case, MCP reduces to FT \(^{(9)}\).

We define a function by

$$F_{\gamma,\lambda}(u) = \begin{cases} u & |u| \geq \gamma \lambda \\ \gamma \lambda & |u| < \gamma \lambda \end{cases},$$

where $\lambda > 0$ and $\gamma > 1$ are parameters. Note that $\gamma \lambda \geq \lambda$ since $\gamma > 1$. The FT estimate in an orthogonal case is given by

$$\beta_k^{FT}(\hat{b}_k) = F_{\gamma,\lambda}(\hat{b}_k).$$

By the definition of $F_{\gamma,\lambda}$, it is easily understood that the estimates with large absolute values are harmless in FT.

We define

$$\hat{K}_{0,\gamma,\lambda} = \{ k : |\hat{b}_k| \geq \gamma \lambda \}$$

and

$$\hat{K}_{1,\gamma,\lambda} = \{ k : \lambda \leq |\hat{b}_k| < \gamma \lambda \}$$

and $\hat{k}_{j,\gamma,\lambda} = |\hat{k}_{j,\gamma,\lambda}|$ for $j = 0, 1$. Since we have

$$\frac{\partial \beta_k}{\partial \hat{b}_k} = \begin{cases} 1 & |u| \geq \gamma \lambda \\ 0 & |u| < \lambda \end{cases},$$

the DOF of FT is given by

$$D_n^{FT}(\gamma) = \sigma^2 E \sum_{k=1}^{n} I_{\gamma,\lambda}(\hat{b}_k) + \sum_{k=1}^{n} I_{\gamma,\lambda}(|\hat{b}_k|)$$

$$= \sigma^2 E \hat{K}_{0,\gamma,\lambda} + \sigma^2 \frac{\gamma}{\gamma - 1} E \hat{K}_{1,\gamma,\lambda}$$

by the Stein’s lemma.

Note that FT connects ST to HT by controlling $\gamma$; i.e. FT goes to ST as $\gamma \to \infty$ and goes to HT as $\gamma \to 1$ in some sense. On the other hand, NG does not have this property. However, as shown in the next section, we can extend NG to bridge the gap between ST and HT. It is a natural extension of ST and can connect to HT by a hyper-parameter.

### E. Adaptive LASSO (AL)

In \(^{(20)}\), adaptive LASSO estimate in an orthogonal case has been given by

$$\beta_k^{AL}(\gamma) = \left( |\hat{b}_k| - \lambda_R / |\hat{b}_k|^\gamma \right) \sign(\hat{b}_k)$$

where $\gamma > 0$ and $\lambda_R > 0$ is a regularization parameter. This can be written as

$$\beta_k^{AL}(\gamma) = \left( 1 - \lambda_R / |\hat{b}_k|^\gamma + 1 \right) \sign(\hat{b}_k).$$

The threshold level is, thus, given by $\lambda = \lambda_R^{1/(\gamma+1)}$ in AL. Therefore, AL is essentially equivalent to NG when $\gamma = 1$ if we choose $\lambda_R = \lambda^2$ under a given $\lambda$. We show sure AL in later section.

### IV. Scaling of soft thresholding estimator

#### A. Scaling of soft thresholding estimator

We focus on a scaling of the ST estimate :

$$\alpha_k S_\lambda(\hat{b}_k),$$

where $\alpha_k \geq 0$. We define

$$\tilde{\omega}_k = \frac{1}{1 - \lambda / |\hat{b}_k|}$$

for $|\hat{b}_k| > \lambda$. It is easy to check that $\tilde{\omega}_k S_\lambda(\hat{b}_k) = \hat{b}_k$ holds for $|\hat{b}_k| > \lambda$. This implies that $\tilde{\omega}_k$ is a scaling value that gives us a hard thresholding estimate when we give an appropriate definition at $\lambda$. If $|\hat{b}_k| > \lambda$ then we have

$$\tilde{\omega}_k = 1 + \left( \lambda / |\hat{b}_k| \right) + \left( \lambda / |\hat{b}_k| \right)^2 + \left( \lambda / |\hat{b}_k| \right)^3 + \cdots$$

by the Taylor expansion. This implies that the NG estimate is obtained by the first order approximation of $\tilde{\omega}_k$ when we regard the NG estimate as a scaling of the ST estimate. We consider the $m$th order approximation of $\tilde{\omega}_k$ and employ

$$\tilde{\alpha}_{k,m} = \left( 1 + \sum_{j=1}^{m} \lambda^j / |\hat{b}_k|^j \right) \frac{|\hat{b}_k|}{|\hat{b}_k|} \geq \lambda \frac{|\hat{b}_k|}{|\hat{b}_k|}$$

as a scaling value. This is well defined for $\tilde{\omega}_k \geq \lambda$ if $m < \infty$. If $|\hat{b}_k| \geq \lambda$ then it is easy to check that

$$\tilde{\alpha}_{k,m} S_\lambda(\hat{b}_k) = \tilde{\omega}_k - \frac{\lambda}{b_k} \frac{\lambda^m}{|\hat{b}_k|^{m-1}}$$

holds for $m \geq 1$. If $m$ is odd then we simply have

$$\tilde{\alpha}_{k,m} S_\lambda(\hat{b}_k) = \tilde{\omega}_k - \frac{\lambda^{m+1}}{|\hat{b}_k|^{m+1}}$$

if $|\hat{b}_k| \geq \lambda$. We thus have an estimate by

$$\hat{\beta}_{k}^{SST} = \tilde{\alpha}_{k,m} S_\lambda(\hat{b}_k) = \left( 1 - \lambda^{m+1} / |\hat{b}_k|^{m+1} \right) \hat{b}_k$$

when $m$ is odd. We refer to this method as a scaled soft thresholding estimator; i.e. SST estimator for short. Obviously, the SST estimator expands the ST estimator while it shrinks the least squares estimator. As was seen above, SST is consistent with AL if we choose $\lambda_R = \lambda^{1+1}$ in AL. Therefore, SST is
an another implication of AL, in which a hyper parameter in AL corresponds to the order of expansion of scaling values of ST. We denote the DOF for SST by $D_{n}^{\text{SST}}(\lambda)$. Since we have

$$\begin{align*}
\frac{\partial D_{n}^{\text{SST}}}{\partial b_{k}} &= \begin{cases}
1 + m\lambda^{m+1}\hat{b}_{k}^{m+1} & |\hat{b}_{k}| \geq \lambda, \\
0 & |\hat{b}_{k}| < \lambda,
\end{cases}
\end{align*}$$

we obtain

$$D_{n}^{\text{SST}}(\lambda) = D_{1,n}^{\text{SST}}(\lambda) + D_{2,n}^{\text{SST}}(\lambda)$$

by the Stein’s lemma, where

$$D_{1,n}^{\text{SST}}(\lambda) = \sigma^{2} \sum_{k=1}^{n} E_k I_{\lambda}(\hat{b}_{k}) = \sigma^{2} E_{\hat{K}_{\lambda}}$$

$$D_{2,n}^{\text{SST}}(\lambda) = \sigma^{2} \sum_{k=1}^{n} m E_k \left(\frac{\lambda}{\hat{b}_{k}}\right)^{m+1} I_{\lambda}(\hat{b}_{k})$$

$$= \sigma^{2} m E \sum_{k \in \hat{K}_{\lambda}} \left(\frac{\lambda}{\hat{b}_{k}}\right)^{m+1}$$

(44)

when $m$ is odd. In (44), we define that the sum is zero if $\hat{K}_{\lambda}$ is empty. Note that if we set $\lambda = \lambda^{1/(\gamma+1)}$ then $D_{n}^{\text{SST}}(\lambda)$ is the DOF of AL.

B. Discussion on SST

SST includes ST if $m \geq 1$. SST reduces to formally ST if $m = 0$ and it reduces to a naive NG if $m = 1$. We show the output of HT, ST, NG and SST with $m = 5$ in Fig. 1. It is obvious that, by controlling $m$, SST can be bridge for linking ST and HT in some sense. Note that the first term of $D_{n}^{\text{SST}}(\lambda)$ is the DOF of ST. Therefore, the second term is related to HT. Since the second term is positive, the DOF of SST is larger than that of ST. Since the DOF represents the DOOF, this result says that SST has two sources of over-fitting and the over-fitting is more serious in SST compared to ST. The first source that is originated from the first term is the DOF of ST and, thus, is determined by the number of non-zero coefficient estimates as seen in (19). This is a natural measure of the model complexity, thus the DOOF. The second one that is originated from the second term is related to the property of HT; i.e. other than the property of ST. This does not seem to be a simple form that reflects the model complexity. $(\lambda/\hat{b}_{k})^{m+1}$ is large when $\hat{b}_{k}$ is close to $\lambda$. This is obvious from the fact that the variation of the second term of (39) with respect to $\hat{b}_{k}$ is large when $\hat{b}_{k}$ is close to $\lambda$ with $\lambda \geq |\hat{b}_{k}|$. Since $\hat{b}_{k}$ is locally distributed around $\hat{b}_{k} = E\hat{b}_{k}$, the contribution of the $k$th component is large if $\lambda$ is close to $E\hat{b}_{k}$. This corresponds to the implication of (8) derived by the Stein’s lemma. In other words, if we change $\lambda$ then the impact of the $k$th component is large in $D_{2,n}^{\text{SST}}(\lambda)$ when $\lambda$ is around $\hat{b}_{k}$. Especially, there are many components with $\hat{b}_{k} = 0$ in a sparse setting. As a result, it is expected that $D_{2,n}^{\text{SST}}(\lambda)$ takes a large value when $\lambda$ is close to zero while it may not be straightforward. We consider the behavior of $D_{2,n}^{\text{SST}}(\lambda)$ in detail through the analysis of HT since HT may approximate SST with a large $m$ in some sense.

C. Limit of DOF of SST

Since SST approaches HT as $m \to \infty$ in some sense, we firstly consider the DOF of HT. Then, we discuss the convergence of the DOF of SST to that of HT. The DOF of HT has already been given in (18). We show a simple derivation of the DOF of HT.

$$D_{n}^{\text{HT}}(\lambda) = n \sum_{k=1}^{n} E_k \hat{b}_{k}^{\text{HT}} - b_k).$$

By defining

$$M_{\lambda}(u) = \lambda \left\{ I_{\lambda}(u) - I_{-\infty,-\lambda}(u) \right\},$$

we have

$$H_{\lambda}(u) = S_{\lambda}(u) + M_{\lambda}(u).$$

We then have

$$D_{n}^{\text{HT}}(\lambda) = D_{n}^{\text{ST}}(\lambda) + D_{n}^{\text{HT}}(\lambda),$$

(48)

where

$$D_{2,n}^{\text{HT}}(\lambda) = n \sum_{k=1}^{n} E_k (\hat{b}_{k} - b_k) M_{\lambda}(\hat{b}_{k}).$$

(49)

This is called the “search degrees of freedom” of best subset selection in (18). This may because $M_{\lambda}$ seems to behave as an index function for choosing non-zero components; i.e. subset search. Let $\phi_{\mu,\tau}$ be a probability density function of $N(\mu, \tau^2)$. It is easy to see that

$$\int_{-\infty}^{\lambda} (\xi - \mu) \phi_{\mu,\tau}(\xi) d\xi = \tau^2 \phi_{\mu,\tau}(\lambda)$$

(50)

$$\int_{-\infty}^{\lambda} (\xi - \mu) \phi_{\mu,\tau}(\xi) d\xi = -\tau^2 \phi_{\mu,\tau}(\lambda)$$

(51)

hold. We define

$$h_{\mu,\tau}(\lambda) = \lambda \left( \phi_{\mu,\tau}(\lambda) + \phi_{\mu,\tau}(-\lambda) \right).$$

(52)
Since \( \hat{b}_k \sim N(b_k, \tau_n^2) \) and \( \tau_n^2 = \sigma^2/n \), we then have
\[
D_{2,n}^{HT}(\lambda) = \sigma^2 \sum_{k=1}^{n} h_{b_k, \tau_n}(\lambda)
\]
by (49), (50) and (51). As another expression, by using the Dirac’s delta function, we can write
\[
D_{2,n}^{HT}(\lambda) = \sigma^2 \sum_{k=1}^{n} \mathbb{E}_k \left( \delta(\hat{b}_k - \lambda) + \delta(\hat{b}_k + \lambda) \right).
\]
(54)

The extension of the Stein’s lemma in this direction have been made in [18]. This gives us a natural interpretation in the sense of that of SST. To do this, we just evaluate point here is that the DOF of HT is also decomposed into the decomposition of the DOF; i.e. the DOF of ST and the reminder connecting to HT. This is because SST includes ST as a part of the Taylor expansion. Moreover, the first term that is the DOF of ST is consistent with that of HT. Such an exact and convenient decomposition of the DOF does not appeared in FT. By this result, we can guarantee that the DOF of SST with a large \( m \) is approximated by that of HT.

V. A NUMERICAL EXAMPLE AND DISCUSSIONS

A. Numerical example

We consider a set of \( n \) functions, \( G_n = \{g_1, g_2, \ldots, g_n\} \), in which
\[
g_k(t) = \begin{cases} 
1 & k = 1 \\
\sqrt{2} \cos(kt/2) & k: \text{even and } k \neq 1, n \\
\sqrt{2} \sin(kt/2) & k: \text{odd and } k \neq 1, n \\
\cos(kt/2) & k = n
\end{cases}
\]
(62)

We set \( t_i = 2\pi(i - 1)/n \) for \( i = 1, \ldots, n \), where \( n \) is even. We then choose \( x_{i,j} = g_j(t_i) \). Then, \( X \) is an \( n \times n \) orthogonal matrix.

We here conduct a monte carlo simulation. The result here is partly consistent with the experiment in [18]; i.e. the result for HT. We generate samples according to (1) under the condition below. We employ the above design matrix. We set \( K^* = \{1, 2, 3, 4, 5\} \) and \( b_k = 1, k = 1, 2, 3, 4, 5 \) for a true representation. We set \( \sigma^2 = 1 \) for a Gaussian additive noise. We set \( n = 256 \). We then estimate the coefficients by using HT, ST and SST with \( m = 21 \) under a fixed threshold level. Here, we refer to SST with \( m = 21 \) as SST simply. Note that \( m = 21 \) may be large enough for approximating HT.

For the coefficient estimates, we calculate SURE and an actual risk. The latter is calculated by the squared error sum between the estimated outputs and true outputs. We repeat this procedure for \( S = 5000 \) times and calculate the averages of SUREs and actual risks at a fixed threshold level. We conduct this procedure for candidates of the threshold level, \( \lambda \in \{0.01, 0.02, \ldots, 0.1, 0.15, 0.2, \ldots, 1.2, \ldots, 10\} \).

The results are summarized in Fig2. Fig2(a) shows the first and second terms of the DOF of SST, the entire DOF of SST and the theoretical value of the second term for HT. Fig2(b) shows the risks for HT, ST and SST together with SUREs for ST and SST. We explain the validity of this result below.

B. Discussion on DOF

In Fig2(a), we can see that the first term of DOF decreases as the threshold level, \( \lambda \), increases. This indicates that the DOF of ST as [19] says. On the other hand, the second term of the DOF of SST is almost consistent with the theoretical
value for HT. This supports our theoretical result for a large $m$ in SST above. The important point in Fig. 2 (a) is the non-monotonicity of the second term of DOF for SST. It is a different property seen in ST and is mentioned in [18]. We next consider this point for HT, thus SST with a large $m$.

Here, we remind the definition of $K^* = \{ k : b_k \neq 0 \}$ and $K^+ = |K^*|$. We consider a sparse and large sample case, in which $k^* \ll n$ and $n$ is large. In this setting, $\tau_n^2 = \sigma^2/n$ that is the variance of $\tilde{b}_k$ is small since $n$ is large. By (52), it is easy to see that $h_{0,\tau_n}(\lambda) \geq 0$ and

$$h_{0,\tau_n}'(\lambda) = 2 \left( 1 - \frac{\lambda^2}{\tau_n^2} \right) \phi_{b_k,\tau_n}(\lambda)$$

holds; e.g. see also [18]. Therefore, for components with zero true coefficients, $h_{0,\tau_n}$ increases for $\lambda < \tau_n$ and decreases for $\lambda > \tau_n$ as $\lambda$ increases; i.e. the peak occurs at $\lambda = \tau_n$. This non-monotonicity of the DOF is a different property seen in ST and is mainly mentioned in [18]. We now step into the analysis of the DOF of HT under a sparse, large sample and non-parametric setting. We consider the case where $\lambda = \tau_n$. If we define $S_1(\lambda) = \sum_{k \in K^*} h_{b_k,\tau_n}(\lambda)$ and $S_2(\lambda) = \sum_{k \in K^+} h_{b_k,\tau_n}(\lambda)$ then $D^H(\lambda) = \sigma^2 (S_1 + S_2)$. $S_1$ and $S_2$ are due to the non-zero true components and zero true components respectively. We roughly evaluate $S_1(\tau_n)$ and $S_2(\tau_n)$ in a sparse and large sample setting. If $k \in K^*$ then we have $\tau_n (\phi_{b_k,\tau_n}(\tau_n) + \phi_{b_k,\tau_n}(\tau_n)) \approx C_1 e^{-nC_2}$ for positive constants $C_1$ and $C_2$ since $\tau_n = \sigma / \sqrt{n} \ll |b_k|$. We thus have $S_1(\tau_n) \approx k^* C_1 e^{-nC_2}$. On the other hand, if $k \in K^+$ then $\tau_n \phi_{b_k,\tau_n}(\tau_n) = C_3$ for a positive constant $C_3$. We thus have $S_2(\tau_n) = 2(n-k^*)C_3 \approx 2n C_3$ in a sparse setting. Therefore, we have $S_1(\lambda) \ll S_2(\lambda)$ at $\lambda = \tau_n$; i.e. the impact of zero true components dominates those of non-zero true components around $\lambda = \tau_n$. The impact of the zero true coefficients monotonically decreases as $\lambda$ increases for $\lambda \geq \tau_n$. For example, if we define $\lambda_n = \sqrt{2k\tau_n \log n/n}$ and set $\lambda = \lambda_n$, then $\tau_n (\phi_{b_k,\tau_n}(\lambda_n) + \phi_{b_k,\tau_n}(\tau_n)) \approx C/n$ for a positive constant $C$. Therefore, we have $S_2(\lambda_n) \approx 2C$ which is very smaller than $S_2(\tau_n)$. For the non-zero true components, if $\lambda$ is around $|b_k| \neq 0$ then either $\phi_{b_k,\tau_n}(\lambda)$ or $\phi_{b_k,\tau_n}(\tau_n)$ is large. Therefore, $S_1(\lambda)$ can be large around $\lambda = |b_k|$. If $\lambda = |b_k|$ then $h_{b_k,\tau_n}(\lambda) \approx C / \sqrt{n}$ for a positive constant $C$. However, if $\lambda = |b_k| \pm \epsilon$ for $\epsilon > 0$ then $h_{b_k,\tau_n}(\lambda) \approx \sqrt{n} C_1 e^{-nC_2}$ for positive constants $C_1$ and $C_2$. Therefore, the impact of a non-zero true coefficient is point-wise. Additionally, it is a single contribution at only around $\lambda = |b_k| \neq 0$; i.e. in general, $b_k, k \in K^*$ take different values. This is different from a mass and large effect of zero true components at around $\lambda = \tau_n$.

As a result, we can say that the effect of the second source of over-fitting in HT and, thus SST with a large $m$ can be large around $\lambda = \tau_n$ in a sparse and large sample setting. And it is brought about by estimates of zero true components. In our setting of the numerical example, we have $\tau_n = \sqrt{\sigma / \sqrt{n}} = 0.0625$ and the second term is maximized at around this value in Fig. 2 (a). This is an evidence for our discussion above. Note that $\tau_n = \sigma / \sqrt{n}$ is small in a large sample case. Therefore, the second term is relatively large for small value of $\lambda$. Actually, it dominates the first term at around $\lambda = \tau_n$ in Fig. 2 (a). The entire DOF of SST is relatively large for small value of $\lambda$. This implies that the DOF is serious for SST compared to ST when the threshold level is small. The important point is that this effect is mainly brought about by the zero true coefficients under a sparse setting in a nonparametric regression. Therefore, the over-fitting behavior of SST is notably different from that of ST around $\lambda = \tau_n$. From the another point of view, ST suppresses this effect by an amount of shrinkage even when the selection via thresholding is the same as the manner of HT.

![Fig. 2. The results of monte carlo simulation. (a) The first and second terms of the DOF of SST, the entire DOF of SST and the theoretical value of the second term for HT. We set $m = 21$ for SST in this simulation. (b) Risks for HT, ST and SST together with SUREs for ST and SST.](image-url)
second term at around $\lambda = 0$ and also $\lambda = 1$. The former is due to zero true coefficient values and the latter is due to non-zero true coefficient values; i.e. $b_k = 1$ for all $k \in K^*$.  

C. Discussion on risk

In Fig 2 (b), firstly, we can see that SURE is almost consistent with the actual risk for ST and SST. Moreover, the risk and SURE of SST approximate the risk of HT well. These two facts support our theoretical result. We next consider the difference between ST and SST.

As well known, HT and the bridge methods can reduce the bias that arises in ST. This bias problem occurs because both of the threshold level and the amount of shrinkage are simultaneously controlled by a single parameter. The bias harms the estimates of non-zero true components and causes a high risk. Although this may interfere with the consistency of thresholding; e.g. see [20], [21], it is free for our orthogonal high risk. Although this may interfere with the consistency of selection based on the risk that is a prediction error. As found in Fig 2 (b), the risks of HT and SST are minimized at around $\lambda = 0.5$ while the risk of ST is large at around this value. This is because of the bias mentioned above. The important point is that, in ST, a threshold level that minimizes the risk tends to be small due to the bias problem.

On the other hand, for small threshold values, the risks of all methods are high. As easily understood, this is because the over-fitting to noise. At a very small threshold levels, risks are very high for all methods due to the over-fitting originated from the number of unremoved coefficients. The important point is that the risks of HT and SST is higher than that of ST. The difference is notable at around $\tau_0$ and $\frac{1}{2}$, which is around $\tau_0$. This fact corresponds to a high DOOF due to a HT property as was found in Fig 2 (a). We can regard $\tau_0$ as a noise level for the coefficient estimate in some sense. Therefore, we can say that the risks of HT and SST are high at around the noise level. Although this is caused by over-fitting, it may be preferable in model selection based on a risk estimate because a high risk at around a noise level avoids the choice of a excessively larger model that is in over-fitting.

As a result, SURE tends to choose a larger model for ST and a smaller model for HT and SST. Note that, for a sparse and non-parametric setting, a penalty for over-fitting is very high at around noise level in HT and SST. Therefore, those may appropriately remove noise components in a prediction error based model selection.

D. Model selection properties

We here compare HT, ST, FT and SST in terms of risk, sparseness and consistency of selection. We generate samples according to (1) under the condition below. We set $n = 256$ and $\sigma^2 = 1$. We consider the two case of a true representation.

Case-1 $K^* = 1, 2, 3, 4, 5$ and $b_k = 1$ for $k \in K^*$.  
Case-2 $K^* = 1, 2, \cdots, 64$ and $b_k = \frac{5}{k}$ for $k \in K^*$.

The first case assumes that a true representation is very sparse and it can be easily identified. The second case assumes that a true representation is moderately sparse while some components are difficult to be identified. For each case, we estimate the coefficients by using HT, ST, FT and SST under a fixed threshold level. For HT, we employ the universal thresholding level [4], [5]. We need the estimates of noise variance for computing SURE and threshold level of HT. It is calculated by an unbiased estimate using the first $n/2$ components. It is possible because of the setting of $K^*$. However, we note that it is difficult to obtain an unbiased estimate in general situations while a suitable solution is give in wavelet denoising [4], [5]. The candidates of the threshold level are $\lambda \in \{0.02, 0.03, \ldots, 0.1, 0.2, \ldots, 1\}$. FT and SST have additional hyper-parameters $\gamma$ and $m$ respectively. The candidate of these parameters are $\gamma \in \{1, 1.2, 1.5, 2, 3, 4, 5\}$ and $m \in \{1, 3, 5, 7, 9, 11\}$ respectively. We choose a threshold level according to SURE for HT and ST. For FT and SST, we choose both of threshold level and hyper-parameter by a grid search of SURE. Since we know the true representation, we can calculate an actual risk. For comparing model selection properties, we obtain the number of non-zero coefficient estimates. Note that it is a measure of sparseness. Also, we measure a selection error by the cardinality of the symmetric difference between $K^*$ and $\hat{K}_\lambda$. We refer to these as Risk, $\hat{k}$ and SErr here. We repeat $S = 5000$ trials and calculate the averages of these values. In Table I, we show the result, in which we also append the standard deviation in the bracket. We summarize the results.

- For Case-1, HT is superior to the other methods in terms of all of risk, sparseness and consistency. On the other hand, ST shows the worst performance that is caused by a large bias for contributed coefficient estimates. This induces a choice of a larger size as suggested by Fig 2. SST and FT are inbetweens. Since a true representation is clearly identified in Case-1, it is easy to separate it from noise. The success of HT comes from this fact.
- For Case-2, ST gives the lowest risk while it does not give us a sparse and correct representation. On the other hand, HT shows the worst risk value while it gives a highly sparse representation. This comes from the fact that there are many true non-zero coefficients that are hard to be

| TABLE I | THE AVERAGES OF RISK, $\hat{k}$ AND SERR. |
|----------|----------------------------------------|
|          | (a) Case-1                             | (b) Case-2                        |
|          | Risk                                   | $\hat{k}$                         | SErr                   |
| HT       | 0.0390 (0.0257)                        | 5.2098 (0.4707)                   | 0.2090 (0.4707)        |
| ST       | 0.0164 (0.0406)                        | 39.2140 (2.6461)                  | 34.2140 (2.6461)       |
| FT       | 0.0006 (0.1199)                        | 9.2940 (0.0369)                   | 4.2940 (0.0369)        |
| SST      | 0.0384 (0.0651)                        | 7.1930 (0.1393)                   | 2.1930 (0.1393)        |

(a) Case-1

|          | Risk                                   | $\hat{k}$                         | SErr                   |
| HT       | 0.0786 (0.1058)                        | 26.3850 (3.1456)                  | 37.0290 (3.0498)       |
| ST       | 0.0590 (0.0960)                        | 126.7680 (20.1390)                | 77.7920 (15.8806)      |
| FT       | 0.0306 (0.1529)                        | 84.2550 (20.1394)                 | 41.0240 (15.5550)      |
| SST      | 0.0600 (0.1191)                        | 81.0050 (17.8694)                 | 44.6370 (11.4952)      |

(b) Case-2
identified due to their magnitudes. Of course, the hardness may depend on a signal to noise ratio and the number of samples. HT tends to remove these weak components. SErr is relatively small for HT since HT may surely select the true components. We can see that ST may select redundant components while it gives a low risk. This is because many true components are included in the selected components. Again, SST and FT are inbetween.

By these results, SST and FT may be reliable in applications since we do not know the situation of a true representation. The performances of SST and FT are comparable. A certain advantage of SST is found in the tables. This may come from the fact that FT connects ST to HT by a non-smooth manner while SST does by a smooth manner.

VI. CONCLUSIONS AND FUTURE WORKS

In this article, we developed and analyzed SST method in which ST estimators are independently expanded by empirical scaling values. The scaling values have a common hyper-parameter that is an order of Taylor expansion of an ideal scaling value that achieves HT. The SST estimator expands the ST estimator while it shrinks the least squares estimator. SST estimator is a bridge estimator between ST and HT estimators and is a generalized estimator that includes ST and NNG estimators as special cases. It also gives another derivation of the well-known AL under a specific regularization parameter and, therefore, it gives an interpretation of AL.

We then derived the DOF of SST estimator by means of the SURE and found that it is decomposed into the DOF of ST and the reminder connecting to HT. In this meaning, SST method gives a natural bridge between ST and HT. Since the DOF represents the DOOF, this result implies that there are two sources of over-fitting in SST method. The first source originated from ST is determined by the number of un-removed coefficients and is a natural measure of the DOOF. Since we showed that the DOF of SST converges to that of HT as the expansion order goes to infinity, we attempt to analyze the second source of HT as a limit case. To do this, we showed a simple numerical example and explained the numerical result based on the theoretical result. In this example, we showed the change of DOF, risk and SURE in terms of threshold levels. We here could see the non-monotonicity of the second source of over-fitting in DOF as pointed out in [13]. We then found the non-monotonicity at a relatively small threshold level comes from a over-fitting to noise. More precisely, in a sparse and non-parametric setting, the second source of over-fitting is largely determined by coefficient estimates whose true values are zeros. And, the impact is maximized when a threshold level is at around noise levels in these coefficient estimates. This excess over-fitting given by the second source leads to a large penalty in risk. Therefore, for ST, a larger model that is in over-fitting tends to be excluded in a model selection based on a risk estimate. On the other hand, as well known, for a large threshold level, risk of ST is high due to a bias problem and SST are free from this. As a result, SURE for ST tends to choose a smaller threshold level that yields a larger model while SURE for SST tends to choose a larger threshold level that yields a smaller model. In an actual model selection experiment, we showed that advantage of thresholding method depends on the signal-to-noise ratio and the bridge method such as SST and FT may be preferable compared to ST and HT in general situations.

On the other hand, in thresholding methods, coefficients with large contribution to fitting are not removed or, more actively, selected to reduce the fitting error in greedy manner. Obviously, this can be a source of over-fitting and it may be independent of model size; i.e. the number of coefficients. Indeed, a detailed asymptotic analysis in this direction is found in [16], in which the over-fitting mechanism in a greedy method is shown to be related to the extreme value property of the coefficient estimates of zero true values. This is partly consistent with our result here. As a future work, we may need more detailed correspondence between the result here and the results in [16] that focus on the selectability of variables in the fitting procedure. This point may be a part of the answer for an exploration in [13].

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