A COMMENT ON STEIN’S UNBIASED RISK ESTIMATE FOR REDUCED RANK ESTIMATORS

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Abstract. In the framework of matrix valued observables with low rank means, Stein’s unbiased risk estimate (SURE) can be useful for risk estimation and for tuning the amount of shrinkage towards low rank matrices. This was demonstrated by Candès et al. (2013) for singular value soft thresholding, which is a Lipschitz continuous estimator. SURE provides an unbiased risk estimate for an estimator whenever the differentiability requirements for Stein’s lemma are satisfied. Lipschitz continuity of the estimator is sufficient, but it is emphasized that differentiability Lebesgue almost everywhere isn’t. The reduced rank estimator, which gives the best approximation of the observation with a fixed rank, is an example of a discontinuous estimator for which Stein’s lemma actually applies. This was observed by Mukherjee et al. (2015), but the proof was incomplete. This brief note gives a sufficient condition for Stein’s lemma to hold for estimators with discontinuities, which is then shown to be fulfilled for a class of spectral function estimators including the reduced rank estimator. Singular value hard thresholding does, however, not satisfy the condition, and Stein’s lemma does not apply to this estimator.

1. Introduction

Let $Y$ be an $p \times q$ matrix with $p \geq q$ and singular value decomposition

$$Y = \sum_{k=1}^{q} d_k u_k v_k^T.$$ 

If all the singular values are unique and ordered as $d_1 > d_2 > \ldots > d_q \geq 0$ the rank $r$ approximation of $Y$ that minimizes the Frobenius norm error is given by

$$\hat{\mu}(r) = \sum_{k=1}^{r} d_k u_k v_k^T,$$

for $r \in \{1, \ldots, q - 1\}$. The hard threshold approximation given by

$$\overline{\mu}(\lambda) = \sum_{k=1}^{q} d_k 1(d_k \geq \lambda) u_k v_k^T$$

for $\lambda \geq 0$ yields the same sequence of approximations but parametrized differently.

If $Y = (Y_{ij})_{i,j}$ has independent entries with

$$Y_{ij} \sim \mathcal{N}(\mu_{ij}, \sigma^2)$$

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and \( \mu = (\mu_{ij})_{i,j} \) is of low rank, the approximations \( \hat{\mu}(r) \) or \( \overline{\mu}(\lambda) \) are sensible estimators of \( \mu \) for suitable choices of \( r \) or \( \lambda \). Both estimators are examples from the more general class of spectral function estimators

\[
\hat{\mu} = \sum_{k=1}^{q} f_k(d_k) u_k v_k^T, \quad \lambda_1 > \lambda_2 > \ldots > \lambda_q \geq 0
\]

for some spectral functions \( f_k : [0, \infty) \to [0, \infty) \). The hard thresholding estimator has \( f_k(d) = d 1(d \geq \lambda) \), and the estimator with \( f_k(d) = d 1(k \leq r) \), which gives the best rank \( r \) approximation, will be referred to as the reduced rank estimator.

In the framework of spectral function estimators, Candès et al. (2013) derive an explicit formula (formula (9) in their paper) for the divergence of the estimator when \( Y \) has distinct singular values and \( f_k \) is differentiable in a neighborhood of \( d_k \). This divergence is required for the computation of SURE, and it’s therefore important for applications. They also demonstrate in detail (Lemma III.3) how Stein’s lemma applies in the special case of soft thresholding, which is a spectral function estimator with all spectral functions equal to the continuous function \( f_k(d) = (d - \lambda)_+ \). Candès et al. (2013) further show that the divergence extends continuously to all matrices (Theorem IV.6) whenever all spectral functions are identical and sufficiently smooth. That result doesn’t apply to the hard thresholding estimator (though the spectral functions are identical, they are discontinuous) or to the reduced rank estimator (the spectral functions are not all identical).

Mukherjee et al. (2015) derive similar formulas for the divergence – apparently unaware of the paper by Candès et al. (2013). One difference is that Mukherjee et al. (2015) focus on the regression setup, where the columns of the observation matrix are projected onto a fixed subspace before it is subjected to a low rank approximation.

Neither Candès et al. (2013) nor Mukherjee et al. (2015) provides conditions for general spectral function estimators that ensure that Stein’s lemma applies. Mukherjee et al. (2015) indicate on page 460 that the mere existence of the partial derivatives (Lebesgue) almost everywhere is sufficient for Stein’s lemma, which is not the case as shown below. Candès et al. (2013) state a correct version of Stein’s lemma as their Proposition III.1, which (correctly) assumes weak differentiability of the estimator. Weak differentiability of the soft threshold estimator is then shown in detail (using that it’s Lipschitz), but Candès et al. (2013) don’t clarify if e.g. their Theorem IV.6 implies the required weak differentiability for more general spectral function estimators. The theorem does not cover the reduced rank estimator anyway.

The purpose of this note is to provide conditions ensuring that a spectral function estimator is, indeed, weakly differentiable so that Stein’s lemma applies. In particular, we show that the reduced rank estimator is weakly differentiable so that the SURE formulas as given by Candès et al. (2013) or Mukherjee et al. (2015) result in unbiased estimation of the risk. To illustrate the relevance of such sufficient conditions, we show by a small simulation that the SURE formula for singular value hard thresholding doesn’t give unbiased estimation of the risk.
2. Stein’s lemma

In this section we state a sufficient condition for Stein’s lemma, which can then be shown to hold for the reduced rank estimator. It’s formulated for \( n \)-dimensional Gaussian vectors and applies to the matrix valued observations and estimators above by taking \( n = pq \).

Let \( y \sim \mathcal{N}(\mu, \sigma^2I) \) be an \( n \)-dimensional Gaussian random variable and \( \hat{\mu} \) an estimator of \( \mu \) with finite second moment; \( E[||\hat{\mu}||^2_2] < \infty \). For such an estimator, Stein’s lemma or Stein’s identity (Lemma 1 or Lemma 2 in Stein (1981)) implies that

\[
\frac{1}{\sigma^2} \sum_{i=1}^{n} \text{cov}(\hat{\mu}_i, y_i) = \sum_{i=1}^{n} E(\partial_i \hat{\mu}_i) = E(\nabla \cdot \hat{\mu}) \tag{1}
\]

provided that \( \hat{\mu} \) is almost differentiable and

\[
\sum_{i=1}^{n} E|\partial_i \hat{\mu}_i| < \infty. \tag{2}
\]

The quantity

\[
\text{df} = \frac{1}{\sigma^2} \sum_{i=1}^{n} \text{cov}(\hat{\mu}_i, y_i) \tag{3}
\]

is usually referred to as the effective degrees of freedom, and when Stein’s lemma holds, the divergence

\[
\nabla \cdot \hat{\mu} = \sum_{i=1}^{n} \partial_i \hat{\mu}_i
\]

is an unbiased estimate of df. However, if \( \hat{\mu} \) is not continuously differentiable everywhere, care has to be taken to verify almost differentiability even if the divergence \( \nabla \cdot \hat{\mu} \) is well defined Lebesgue almost everywhere. Likewise, the moment condition (2) on the derivative must be verified. All conditions for Stein’s lemma are fulfilled if \( \hat{\mu} \) is Lipschitz as shown e.g. by Candès et al. (2013) in their Lemma III.2, but for discontinuous estimators the situation is more complicated.

For example, take \( \hat{\mu} = 1(y \geq 0) \) for \( n = 1 \), then it is straightforward to see that (1) doesn’t hold, though this function is continuously differentiable everywhere except in 0. A “real” estimator for which Stein’s lemma doesn’t apply is the hard threshold estimator, \( \hat{\mu} = y1(|y| \geq c) \), as treated extensively by Tibshirani (2015), and further examples and an extension of Stein’s lemma are given by Mikkelsen & Hansen (2017). Differentiability Lebesgue almost everywhere is generally not sufficient for Stein’s lemma to apply and (1) to hold.

We state below a sufficient condition for (1) to hold that can be verified in the case of reduced rank estimation. To this end let \( \mathcal{H}^{n-1} \) denote the \( (n-1) \)-dimensional Hausdorff measure.
Proposition 1. Let $E \subseteq \mathbb{R}^n$ be a closed set such that

$$\hat{\mu} : E^c \rightarrow \mathbb{R}^n$$

is continuously differentiable, then (1) holds if $\mathcal{H}^{n-1}(E) = 0$ and either (2) is satisfied or $\nabla \cdot \hat{\mu} \geq 0$ Lebesgue almost everywhere.

Proof. We first show that the condition $\mathcal{H}^{n-1}(E) = 0$ implies almost differentiability of $\hat{\mu}$. As pointed out by Johnstone (1998), see also Fourdrinier & Wells (2012) and Candès et al. (2013), the differentiability requirement for Stein’s lemma is effectively that the estimator is weakly differentiable, that is, that it belongs to the Sobolev space $W^{1,1}_{loc}(\mathbb{R}^n)$. This is the case if for all $i$ and Lebesgue almost all $(y_1, \ldots, y_{n-1}) \in \mathbb{R}^{n-1}$ the function

$$t \mapsto \hat{\mu}(y_1, \ldots, y_{i-1}, t, y_{i+1}, \ldots, y_{n-1})$$

is absolutely continuous on compact intervals, see Theorem 4.9.2.2 in Evans & Gariepy (1992). Alternatively, the proofs in Stein (1981) show directly that almost everywhere absolute continuity of the maps (4) implies (1). See also Definition 2 and Lemma 5 in Tibshirani (2015). When $\mathcal{H}^{n-1}(E) = 0$ the projection maps

$$(y_1, \ldots, y_{i-1}, y_i, y_{i+1}, \ldots, y_n) \mapsto (y_1, \ldots, y_{i-1}, y_{i+1}, \ldots, y_{n-1})$$

for $i = 1, \ldots, n$ map $E$ onto Lebesgue null sets by Corollary 2.4.1.1 in Evans & Gariepy (1992). Thus when $\hat{\mu}$ is continuously differentiable on $E^c$, (4) is continuously differentiable, and thus absolutely continuous, Lebesgue almost everywhere.

Having established almost differentiability, (2) then implies (1). In the second half of the proof we show that $\nabla \cdot \hat{\mu} \geq 0$ is an alternative sufficient condition. To this end, note that since the estimator belongs to $W^{1,1}_{loc}(\mathbb{R}^n)$ then, in fact,

$$\sum_{i=1}^{n} \int \hat{\mu}_i(y) \partial_i \psi(y) dy = - \int \nabla \cdot \hat{\mu}(y) \psi(y) dy$$

for all $\psi \in C_c^\infty(\mathbb{R}^n)$.

Let $\varphi$ denote the density for the $\mathcal{N}(\mu, \sigma^2 I)$ distribution. Choose $\kappa \in C_c^\infty(\mathbb{R}^n)$ with $\kappa(y) \in [0, 1]$ and such that $\kappa(y) = 1$ for $||y||_2 \leq 1$. Defining

$$\varphi_n(y) = \varphi(y) \kappa(n^{-1}y),$$

then $\varphi_n \in C_c^\infty(\mathbb{R}^n)$ and

$$\varphi(y) \geq \varphi_n(y) \geq \varphi(y) 1(||y||_2 \leq n) \Rightarrow \varphi(y)$$

for $n \rightarrow 0$. We also observe that

$$\partial_i \varphi_n(y) = (\partial_i \varphi(y)) \kappa(n^{-1}y) + \varphi(y) n^{-1} \partial_i \kappa(n^{-1}y) \rightarrow \partial_i \varphi(y)$$

for $n \rightarrow \infty$. Here we used that $\partial_i \kappa(n^{-1}y) = 0$ for $||y||_2 < n$ and $\kappa(n^{-1}y) \rightarrow 1$ for $n \rightarrow \infty$. Moreover,

$$|\hat{\mu}_i(y) \partial_i \varphi_n(y)| \leq |\hat{\mu}_i(y) - \mu_i(y)| \varphi(y) / \sigma^2 + C |\hat{\mu}_i(y)| \varphi(y)$$
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for some constant $C$, and the right hand side above is integrable. Thus by dominated convergence,

$$\lim_{n \to \infty} \int \hat{\mu}_i(y) \partial_i \varphi_n(y)\,dy = \int \hat{\mu}_i(y) \partial_i \varphi(y)\,dy.$$  

If $\nabla \cdot \hat{\mu}$ is almost everywhere positive, it finally follows by monotone convergence combined with the dominated convergence above that

$$E(\nabla \cdot \hat{\mu}) = \int \nabla \cdot \hat{\mu}(y) \varphi(y)\,dy$$

$$= \lim_{n \to \infty} \int \nabla \cdot \hat{\mu}(y) \varphi_n(y)\,dy$$

$$= -\lim_{n \to \infty} \sum_{i=1}^{n} \int \hat{\mu}_i(y) \partial_i \varphi_n(y)\,dy$$

$$= -\sum_{i=1}^{n} \int \hat{\mu}_i(y) \partial_i \varphi(y)\,dy$$

$$= \frac{1}{\sigma^2} \sum_{i=1}^{n} \int \hat{\mu}_i(y_i) (y_i - \mu_i) \varphi(y)\,dy$$

$$= \frac{1}{\sigma^2} \sum_{i=1}^{n} \text{cov}(\hat{\mu}_i, y_i).$$

\[ \Box \]

3. Reduced rank estimators

With the squared Frobenius norm as loss function, the risk of an estimator $\hat{\mu}$ is

$$E\|\hat{\mu} - \mu\|^2_F = E\|Y - \hat{\mu}\|^2_F - \sigma^2 pq + 2\sigma^2 \nabla \cdot \hat{\mu}.$$  

When Stein’s lemma applies,

$$\text{SURE} = \|Y - \hat{\mu}\|^2_F - \sigma^2 pq + 2\sigma^2 \nabla \cdot \hat{\mu}$$

is an unbiased estimate of the risk.

For spectral function estimators we observe that

$$\|\hat{\mu}\|^2_F = \sum_{k=1}^{q} f_k(d_k)^2.$$  

Hence if $f_k(d) \leq C_k d$ for some constant $C_k$ (e.g. $f_k$ is shrinking the singular values as is the case for reduced rank, and hard and soft thresholding), then

$$\|\hat{\mu}\|^2_F \leq \max_k \{C_k^2 \sum_{k=1}^{q} d_k^2\} = C\|Y\|^2_F,$$

and $\hat{\mu}$ has finite second moment.
Theorem 1. For the reduced rank estimator $\hat{\mu}(r)$, SURE is an unbiased estimate of the risk, and

$$\nabla \cdot \hat{\mu}(r) = pr + \sum_{k=1}^{r} \sum_{l=r+1}^{q} \frac{d_k^2 + d_l^2}{d_k^2 - d_l^2}$$

(5)

whenever $Y$ has $q$ distinct singular values.

Proof. The reduced rank estimator has finite second moment as argued above. We show that the conditions in Proposition 1 are fulfilled. To this end, note that it’s clear from the explicit formula (5) that $\nabla \cdot \hat{\mu}(r) \geq 0$ whenever $Y$ has no identical singular values. As argued below, this happens Lebesgue almost everywhere. Hence what remains is to show that the set of matrices with no identical singular values and the estimator $\hat{\mu}(r)$ defined on this set fulfill the properties of Proposition 1.

Letting

$$E = \{Y \in M(p,q) \mid Y \text{ has two identical singular values}\}$$

it was shown by Mukherjee et al. (2015) that $E$ is a proper subvariety, and it is, in particular, a closed set.

For $Y \in E^c$ with singular value decomposition

$$Y = \sum_{k=1}^{q} d_k u_k v_k^T$$

and $d_1 > d_2 > \ldots > d_q \geq 0$, the reduced rank estimator is given by

$$\hat{\mu}(r) = \sum_{k=1}^{r} d_k u_k v_k^T,$$

for $r \in \{1,\ldots,q-1\}$. An application of e.g. Theorem 5.3 in Serre (2010) to $Y^T Y$ shows that the singular values $d_1,\ldots,d_{q-1}$ as well as $u_1,\ldots,u_{q-1}$ and $v_1,\ldots,v_{q-1}$ are $C^\infty$ on $E^c$, thus $\hat{\mu}(r)$ is $C^\infty$ on $E^c$ for $r < q$. The algebra by Mukherjee et al. (2015) or Candès et al. (2013) gives the actual partial derivatives and thus the divergence of $\hat{\mu}(r)$. It does require a bit of algebra, though, to realize that the divergence formula (9) in Candès et al. (2013) is identical to the formula in Theorem 3 in Mukherjee et al. (2015), which is stated above as (5). See also (6) below.

We complete the proof using Proposition 1 by establishing that $\mathcal{H}^{pq-1}(E) = 0$. To this end we show that the codimension of $E$ is at least 2.

Let $V_r(m)$ denote the Stiefel manifold of $r$-tuples of $k$-dimensional orthonormal vectors in $\mathbb{R}^m$, and introduce $h : V_{q-2}(q) \times V_q(p) \times [0,\infty)^{q-1} \to M(p,q)$ by

$$h((v_k)_k,(u_k)_k,d) = \sum_{k=1}^{q-2} d_k u_k v_k^T + d_{q-1}(u_{q-1} v_{q-1}^T + u_q v_q^T),$$

where the unit vectors $v_{q-1}$ and $v_q$ are chosen (by $h$ and depending on $(v_k)_k$) orthogonal to $v_1,\ldots,v_{q-2}$. The set $E$ is in the image of $h$ because when two singular values are identical the singular value decomposition is not unique, and it is possible to choose an orthogonal transformation such that $v_{q-1}^T$ and $v_q^T$ in the
singular value decomposition are those chosen by the map $h$. The Stiefel manifold $V_r(m)$ has dimension
\[ \dim(V_r(m)) = rm - \frac{1}{2}r(r + 1) \]
as a differentiable manifold. It follows that $E$ locally is contained in the image under a Lipschitz map of a set of dimension
\[ q(q - 2) - \frac{1}{2}(q - 2)(q - 1) + pq - \frac{1}{2}q(q + 1) + q - 1 = pq - 2. \]
It follows from Theorem 2.4.1 in Evans & Gariepy (1992) that $E$ has Hausdorff dimension at most $pq - 2$, whence $\mathcal{H}^{pq-1}(E) = 0$. By Proposition 1 it follows that (1) holds, and the divergence (5) is an unbiased estimate of the degrees of freedom. □

The fact that $E$ is a proper subvariety implies that $E$ has codimension at least 1 and $E$ has Lebesgue measure zero. As argued above, this is not sufficient for Stein’s lemma to hold. The set $E$ needs to be even smaller as expressed by the condition $\mathcal{H}^{pq-1}(E) = 0$ using the Hausdorff measure. Establishing that $E$ has codimension 2 is enough for this condition to be fulfilled.

The argument above is closely related to the long established fact that the set of matrices with repeated eigenvalues in the set of real symmetric matrices has codimension 2. A result credited to Neumann and Wigner, see p. 36 in Lax (2007). It does, however, appear somewhat complicated to determine the codimension of $E$ as a subvariety, see Dana & Ikramov (2006) for the case of symmetric matrices, and we proceeded in the argument above by effectively counting the free parameters in the singular value decomposition instead.

Essentially the same argument as above can be used for spectral function estimators provided that the spectral functions are suitably well behaved.

Theorem 2. Consider a spectral function estimator
\[ \hat{\mu} = \sum_{k=1}^{q} f_k(d_k) u_k v_k^T \]
with finite second moment and with spectral functions fulfilling that $f_1, \ldots, f_{q-1}$ are continuously differentiable on $(0, \infty)$, $f_q$ is continuously differentiable on $[0, \infty)$, $f_k \geq f_l$ for $k < l$ and $f_k' \geq 0$. Then SURE is an unbiased estimate of the risk, and
\[ \nabla \cdot \hat{\mu} = (p - q) \sum_{k=1}^{q} \frac{f_k(d_k)}{d_k} + \sum_{k=1}^{q} f_k'(d_k) + 2 \sum_{k,l=1 \atop k \neq l}^{q} \frac{d_k f_k(d_k)}{d_k^2 - d_l^2} \]
whenever $Y$ has $q$ distinct singular values.

Proof. As written above, the proof is along the same lines as the proof of Theorem 1. The set $E$ has $(pq - 1)$-dimensional Hausdorff measure zero, and on $E^c$ the estimator $\hat{\mu}$ is continuously differentiable – under the differentiability assumptions on the spectral functions – with divergence given by (6). This divergence formula was shown by Candès et al. (2013) and is given as (9) in their paper.
To use Proposition 1 we verify that $\nabla \cdot \hat{\mu} \geq 0$ on $E^c$. Clearly, as $f_k$ is positive and $f_k'$ is also assumed positive, the first two terms in (6) are positive. For the third term we rearrange the double sum as

$$\sum_{k=1}^{q} \sum_{l=k+1}^{q} \frac{d_k f_k(d_k) - d_l f_l(d_l)}{d_k^2 - d_l^2}.$$ 

Using that $d_k > d_l$ for $k < l$, and that this implies that $f_k(d_k) \geq f_k(d_l) \geq f_l(d_l)$, we have that for each term in this double sum

$$\frac{d_k f_k(d_k) - d_l f_l(d_l)}{d_k^2 - d_l^2} \geq \frac{(d_k - d_l) f_l(d_l)}{d_k^2 - d_l^2} \geq 0.$$ 

This completes the proof. \[\square\]

As stated in the proof above, formula (6) is identical to (9) from Candès et al. (2013). An equivalent formula is given in Theorem 4 in Mukherjee et al. (2015). Clearly, $f_k(d) = d1(k \leq r)$ is smooth, whereas $f_k(d) = d1(d \geq \lambda)$ is not, and Theorem 2 doesn’t apply to singular value hard thresholding.

It’s possible that the monotonicity requirements on the spectral functions above can be relaxed, and that (2) can be verified instead of the positivity on the divergence. But this won’t be pursued in this note.

4. Simulation

This section presents the results from a simulation that illustrates the unbiasedness of SURE for reduced rank estimation and singular value soft thresholding, whereas (6) is shown to be a biased estimate of degrees of freedom for singular value hard thresholding.

For the simulation we made $B = 5000$ simulations with $p = q = 21$ and $Y_{ij}^b \sim \mathcal{N}(0,1)$ for $b = 1, \ldots, B$. With

$$Y^b = \sum_{k=1}^{q} d_k^b u_k^b (v_k^b)^T, \quad d_1^b \geq d_2^b \geq \ldots \geq d_q^b \geq 0$$

the singular value decomposition of the $b$th matrix $Y^b = (Y_{ij}^b)_{i,j}$ we computed the three estimators

$$\hat{\mu}_b(r) = \sum_{k=1}^{r} d_k^b u_k^b (v_k^b)^T \quad \text{(reduced rank)}$$

$$\bar{\mu}_b(r) = \sum_{k=1}^{q} d_k^b 1(d_k^b \geq \lambda) u_k^b (v_k^b)^T \quad \text{(hard thresholding)}$$

$$\tilde{\mu}_b(\lambda) = \sum_{k=1}^{q} (d_k^b - \lambda)_+ u_k^b (v_k^b)^T \quad \text{(soft thresholding)}$$
By the definition of the degrees of freedom, (3), the estimate

$$\hat{df}_0(r) = \frac{1}{B} \sum_{b=1}^{B} \text{tr}(\hat{\mu}_b(r)^T(Y^b - \mu))$$

is an unbiased estimate of df for the reduced rank estimator, and similar estimates of df were computed for the other two estimators. Note that such estimates based on the covariance definition are of no use in real applications as they rely on knowledge of the true mean. In this simulation the true mean was $\mu = 0$. 
Estimates based on the divergence were computed for each of the three estimators as follows

\[
\hat{\text{df}}(r) = pr + \frac{1}{B} \sum_{b=1}^{B} \sum_{k=1}^{r} \sum_{l=r+1}^{q} \frac{(d^b_k)^2 + (d^b_l)^2}{(d^b_k)^2 - (d^b_l)^2}
\]

\[
\overline{\text{df}}(\lambda) = \frac{1}{B} \sum_{b=1}^{B} \left( (p - q + 1) \sum_{k=1}^{q} 1(d^b_k \geq \lambda) + 2 \sum_{k=1}^{q} \sum_{k \neq l} (d^b_k)^2 1(d^b_k \geq \lambda) \right)
\]

\[
\tilde{\text{df}}(\lambda) = \frac{1}{B} \sum_{b=1}^{B} \left( (p - q) \sum_{k=1}^{q} \left( 1 - \frac{\lambda}{d^b_k} \right) + \sum_{k=1}^{q} 1(d^b_k \geq \lambda) + 2 \sum_{k \neq l} d^b_k(d^b_k - \lambda) \right)
\]

Note that with

\[
r(\lambda) = \sum_{k=1}^{q} 1(d^b_k \geq \lambda)
\]

it holds that \(\hat{\text{df}}(r(\lambda)) = \overline{\text{df}}(\lambda)\).

The bias estimate is defined as

\[
\hat{\text{bias}}(r) = \hat{\text{df}}(r) - \hat{\text{df}}_0(r)
\]

for the reduced rank estimator and likewise for the other two estimators. For reduced rank and soft thresholding, the bias is zero by the theoretical results.

Figure 1 shows the results of the simulation. It shows clearly that for singular value hard thresholding the bias is non-zero, though it is relatively small. The results for reduced rank and soft thresholding are completely in concordance with the theoretical results that the bias is 0, and with the simulation results presented by Candès et al. (2013) and Mukherjee et al. (2015).

5. Final comments

There is no claim of originality in terms of the estimators considered or the formulas presented for estimating degrees of freedom and computing SURE. These can be found in the papers by Candès et al. (2013) and by Mukherjee et al. (2015). However, neither of these two papers – nor other papers that the author is aware of – gives a complete proof of the fact that Stein’s lemma does apply to the reduced rank estimator. The purpose of this note was to give this proof.

We may note that the reduced rank estimator, \(\hat{\mu}(r)\), and the hard thresholding estimator, \(\overline{\mu}(\lambda)\), provide the exact same sequence of estimators for a given observation when viewed as functions of \(r\) and \(\lambda\), respectively. Yet, for a fixed \(r\) we can by SURE obtain an unbiased risk estimate for \(\hat{\mu}(r)\), while for fixed \(\lambda\), the SURE formula based on the divergence estimate of degrees of freedom doesn’t give an unbiased risk estimate for \(\overline{\mu}(\lambda)\). While this is understandable when the mapping between the two sequences of estimators is data dependent, it also highlights that the parametrization matters when estimators are assessed via their frequentistic risk. When tuning
parameters are selected by minimizing a risk estimate, this leads to the somewhat peculiar phenomenon that different parametrizations can lead to different choices of tuning parameters. Or as is the case here, that one parametrization provides an unbiased risk estimate, while another provides a biased risk estimate, even though the risk estimates are identical.

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