Second Order Stein: SURE for SURE and Other Applications in High-Dimensional Inference

Pierre C. Bellec∗ and Cun-Hui Zhang†
Department of Statistics, Hill Center, Busch Campus, Rutgers University, Piscataway, NJ 08854, USA.
e-mail: pierre.bellec@rutgers.edu; czhang@stat.rutgers.edu

Abstract: Stein’s formula states that a random variable of the form $z^\top f(z) - \text{div} f(z)$ is mean-zero for all functions $f$ with integrable gradient. Here, $\text{div} f$ is the divergence of the function $f$ and $z$ is a standard normal vector. This paper aims to propose a Second Order Stein formula to characterize the variance of such random variables for all functions $f(z)$ with square integrable gradient, and to demonstrate the usefulness of this Second Order Stein formula in various applications.

In the Gaussian sequence model, a remarkable consequence of Stein’s formula is Stein’s Unbiased Risk Estimate (SURE), an unbiased estimate of the mean squared risk for almost any given estimator $\hat{\mu}$ of the unknown mean vector. A first application of the Second Order Stein formula is an Unbiased Risk Estimate for SURE itself (SURE for SURE): an unbiased estimate providing information about the squared distance between SURE and the squared estimation error of $\hat{\mu}$. SURE for SURE has a simple form as a function of the data and is applicable to all $\hat{\mu}$ with square integrable gradient, for example the Lasso and the Elastic Net.

In addition to SURE for SURE, the following statistical applications are developed: (1) Upper bounds on the risk of SURE when the estimation target is the mean squared error; (2) Confidence regions based on SURE and using the Second Order Stein formula; (3) Oracle inequalities satisfied by SURE-tuned estimates under a mild Lipschtiz assumption; (4) An upper bound on the variance of the size of the model selected by the Lasso, and more generally an upper bound on the variance of the empirical degrees-of-freedom of convex penalized estimators; (5) Explicit expressions of SURE for SURE for the Lasso and the Elastic-Net; (6) In the linear model, a general semi-parametric scheme to de-bias a differentiable initial estimator for the statistical inference of a low-dimensional projection of the unknown regression coefficient vector, with a characterization of the variance after de-biasing; and (7) An accuracy analysis of a Gaussian Monte Carlo scheme to approximate the divergence of functions $f : \mathbb{R}^n \to \mathbb{R}^n$.

Key words: Stein’s formula, variance estimate, risk estimate, SURE, SURE for SURE, Lasso, Elastic Net, model selection, variance of model size, de-biased estimation, regression.

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1. Introduction

1.1. Stein’s formula

The univariate version of Stein’s formula reads $\mathbb{E}[Zg(Z)] = \mathbb{E}[g'(Z)]$ where $Z \sim N(0,1)$ and $g$ is absolutely continuous with finite $\mathbb{E}[|g'(Z)|]^1$. In [Ste72], Stein observed that the set of equations $\mathbb{E}[Zg(Z) - g'(Z)] = 0$ for all absolutely continuous $g$ with integrable gradient characterize the standard normal distribution. Stein went on to show that if $\mathbb{E}[Wg(W) - g'(W)]$ is small for a large class of functions $g$, then $W$ is close in distribution to $N(0,1)$, see for instance [Cha14, Proposition 1.1] for a precise statement. Since then, this powerful technique has been used to obtain central limit theorems under dependence; we refer the reader to the book [CGS10] for a recent survey on Stein’s formula and its application to normal approximation.

The multivariate version of Stein’s formula [Ste81] can be described as follows. Let $z = (z_1, ..., z_n) \sim N(0, I_n)$ be a standard normal random vector. Let $f_1, ..., f_n$ be functions $\mathbb{R}^n \to \mathbb{R}$ and denote by $f$ the column vector in $\mathbb{R}^n$ with $i$-th component equal to $f_i$. If each $f_i$ is weakly differentiable with respect to $z_i$ and $\mathbb{E}[|f_i(z)| + |(\partial / \partial z_i)f_i(z)|] < +\infty$ for each $i \in [n]$, then

(1.1) \[ \mathbb{E}[z^\top f(z)] = \mathbb{E}[\text{div } f(z)] \]

holds, where $\text{div} f = \sum_{i=1}^n (\partial / \partial x_i) f_i$ is the divergence of $f$. The central object of the paper is the random variable $z^\top f(z) - \text{div } f(z)$, which is mean-zero in virtue of (1.1). We provide in the next section an exact identity for the second moment of $z^\top f(z) - \text{div } f(z)$ that we termed **Second Order Stein formula**.

1.2. Related work

Iterated Stein formulae have appeared in several works. If $g : \mathbb{R}^p \to \mathbb{R}$ is smooth with compact support, iterating the univariate Stein’s formula directly yields $\mathbb{E}[z_i z_j g(z)] = \mathbb{E}[(\partial / \partial x_j)(\partial / \partial x_i) g(z)]$ for $i \neq j$ as well as $\mathbb{E}[(z_i^2 - 1)g(z)] = \mathbb{E}[(\partial^2 / \partial x_i^2) g(z)]$. This may be succinctly written as

(1.2) \[ \mathbb{E}[(zz^\top - I_n) g(z)] = \mathbb{E}[\nabla^2 g(z)] \]

where $\nabla^2 g$ is the Hessian of $g$. Formulae that relate $\mathbb{E}[\nabla^2 g(z)]$ to expectations involving $g(z)$ and the density of $z$ have been obtained for non-Gaussian $z$, see [JSA14, Theorem 1], [Erd16], [YBWL, Theorem 2.2] among others. In these works, (1.2) is used to estimate the Hessian in optimization algorithms [Erd16], to estimate the index in some single-index models [YBWL] or to extract discriminative features for tensor-valued data [JSA14]. If $z \sim N(0, I_n)$, the second order iterated Stein formula from these works reduce to (1.2). The

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1. Existence of $\mathbb{E}[Zg(Z)] < +\infty$ follows from $\mathbb{E}[|g'(Z)|] < +\infty$. Indeed by Fubini’s theorem $\mathbb{E}[\max(Z,0)\{g(Z) - g(0)\}] \leq \int_0^\infty |g'(u)| \mathbb{E}[Z1_{Z > u}] du = \mathbb{E}[1_{Z > 0}|g'(Z)|]$ and similarly for $Z < 0$. The
fact that iterating Stein’s formula introduces higher order derivatives should be expected, because Stein’s formula is intrinsically an integration by parts—Stein’s formula is sometimes referred to as Gaussian integration by parts, for instance in [Tal10, Appendix A.4] where statistical physics results are rigorously derived using Stein’s formula and the so-called Smart path method as a central tool. As we will see throughout the paper, the identity for the variance of $z^\top f(z) - \text{div} f(z)$, given in (2.3) below, does not involve the second derivatives of $f$ or require their existence, in striking contrast to the iterated formula (1.2). Although both identities can be seen as second order Stein formulae, they are of a different nature and aim different applications.

1.3. Motivations

In the Gaussian sequence model where $y = \mu + \varepsilon$ is observed for an unknown mean $\mu \in \mathbb{R}^n$ and noise $\varepsilon \sim N(0, I_n)$, Stein’s Unbiased Risk Estimate (SURE), proposed in [Ste81], provides an unbiased estimator for the risk $\|\hat{\mu} - \mu\|^2$ of any estimator $\hat{\mu}(y)$ with integrable gradient as a consequence of (1.1). Namely, the decomposition

$$\|y - \hat{\mu}\|^2 + 2 \text{div} \hat{\mu} - n - \|\hat{\mu} - \mu\|^2 = \varepsilon^\top h(\varepsilon) - \text{div} h(\varepsilon)$$

SURE

where $h(\varepsilon) = \varepsilon - 2(\hat{\mu} - \mu)$ shows that SURE defined above is an unbiased estimate of $E[\|\hat{\mu} - \mu\|^2]$ in virtue of Stein’s formula (1.1) applied to $h$. Although the identity $E[\text{SURE}] = E[\|\hat{\mu} - \mu\|^2]$ is well understood and widely used, little is known about the quality of the approximation $\text{SURE} \approx \|\hat{\mu} - \mu\|^2$ in probability, or equivalently about the variance and concentration properties of the random variable $\varepsilon^\top h(\varepsilon) - \text{div} h(\varepsilon)$ above. A first motivation of the present paper is to understand the stochastic behavior of $\varepsilon^\top h(\varepsilon) - \text{div} h(\varepsilon)$ (beyond unbiasedness) in order to provide uncertainty quantification for SURE. If multiple estimators $\{\hat{\mu}^{(1)}, \ldots, \hat{\mu}^{(m)}\}$ are given for estimation of $\mu$, it is natural to use the estimator among those with the smallest SURE. However, statistical guarantees for such SURE-tuned estimate are lacking, except in very special cases, for instance when $\{\hat{\mu}^{(1)}, \ldots, \hat{\mu}^{(m)}\}$ are linear functions of $y$. When the estimators are linear, SURE is the same as Mallows’ $C_p$ [Mal73] and the SURE-tuned estimate enjoys oracle inequalities with remainder term growing with $\log m$, cf. [Bel18] or Section 3.3 and the references therein. We are not aware of oracle inequalities satisfied by the SURE-tuned estimate for general non-linear estimators $\{\hat{\mu}^{(1)}, \ldots, \hat{\mu}^{(m)}\}$; as explained in Section 3.3 below, our bounds on the variance of $\varepsilon^\top h(\varepsilon) - \text{div} h(\varepsilon)$ are helpful to fill this gap.

A second motivation of the paper regards the Lasso $\hat{\beta}$ in sparse linear regression with Gaussian noise $\varepsilon \sim N(0, I_n)$. Despite an extensive body of literature on the Lasso in the last two decades, little is known about the stochastic behavior of the size of the model selected by Lasso, for instance no previous results are available on the variance of this integer valued random variable. It is well known that the model size of the lasso can be written as
div \, f(\varepsilon) \) for certain function \( f : \mathbb{R}^n \to \mathbb{R}^n \), see Section 3.4 below and the references therein. This integer valued random variable—the size of the model selected by the Lasso—is not differentiable with respect to \( \varepsilon \) and the Stein formulae (1.1)-(1.2) cannot be iterated further to understand the variance of this discrete random variable. Another avenue to bound the variance of a random variable of the form \( g(z), z \sim N(0, I_n) \) is the Gaussian Poincaré inequality, which states that \( \text{Var}[g(z)] \leq \mathbb{E}[\|\nabla g(z)\|^2] \) for differentiable \( g : \mathbb{R}^n \to \mathbb{R} \) [BLM13, Theorem 3.20]. Again, this is unhelpful if \( g(\cdot) \) is discrete-valued and non-differentiable.

1.4. Contributions

The central result of the paper states that the variance of the random variable \( z^\top f(z) - \text{div} f(z) \) is exactly given by

\[
\mathbb{E}[(z^\top f(z) - \text{div} f(z))^2] = \mathbb{E}[\|f(z)\|^2 + \text{trace} ( (\nabla f(z))^2 )]
\]

when both \( f : \mathbb{R}^n \to \mathbb{R}^n \) and its derivative are square integrable. Surprisingly, although this is obtained by iterated integration by parts, the second derivatives do not appear. As explained in the next section, the second derivatives of \( f \) need not exist for the previous display to hold—in that sense, the previous display is more broadly applicable than (1.2). The above formula appears especially useful for estimators commonly called for in high-dimensional statistics such as the Lasso, the Elastic-Net or the Group-Lasso that are differentiable almost everywhere with respect to the noise, but not twice-differentiable. The contributions of the paper are summarized below.

- We derive in Section 2.1 the above Second Order Stein formula, an identity for the variance of the random variable \( z^\top f(z) - \text{div} f(z) \).
- As a consequence, Section 2.3 provides an identity and an upper bound for \( \text{Var}[z^\top f(z) - \text{div} f(z) - g(z)] \) in general, including \( \text{Var}[\text{div} f(z)] \).

Statistical applications are then provided in Section 3:

- Section 3.1 leverages the Second Order Stein formula to construct an unbiased risk estimate for Stein’s Unbiased Risk Estimate (SURE) in the Gaussian sequence model. We shall call this general method SURE for SURE.
- Section 3.2 describes confidence regions based on SURE and the Second Order Stein formula.
- Section 3.3 provides oracle inequalities for SURE-tuned estimates.
- Section 3.4 provides new bounds on the variance of the size of the model selected by the Lasso in sparse linear regression.
- Section 3.5 provides SURE for SURE formulas for the Lasso and E-net as well as the consistency of SURE for SURE in the Lasso case.
- Section 3.6 provides a scheme to de-bias a general class of estimators in linear regression where one wishes to estimate a low-dimensional projection of the unknown regression coefficient vector.
Section 3.7 develops a Monte Carlo scheme to approximate the divergence of a general differentiable estimator when the analytic form of the divergence is unavailable.

The above statistical applications are obtained as consequences of the Second Order Stein formula of Section 2.1. The point of the Second Order Stein formula is that, in many statistical applications where the random variable $z^\top f(z) - \text{div} f(z)$ appears, the standard deviation $\text{Var}[z^\top f(z) - \text{div} f(z)]^{1/2}$ is of smaller order than either $\text{div} f(z)$ or $z^\top f(z)$ and the approximation $z^\top f(z) \approx \text{div} f(z)$ holds not only in expectation as in (1.2), but also in probability.

1.5. Notation

Throughout the paper, $\| \cdot \|$ is the Euclidean norm and $\| \cdot \|_F$ the Frobenius norm, and $f : \mathbb{R}^n \to \mathbb{R}^m$ is L-Lipschitz if $\|f(u) - f(v)\| \leq L \|u - v\|$, $\forall u, v$. For $f : \mathbb{R}^n \to \mathbb{R}^n$ with components $f_i$, denote by $\nabla f_i \in \mathbb{R}^n$ the gradient of each $f_i$, and by $\nabla f$ the matrix in $\mathbb{R}^{n \times n}$ with columns $\nabla f_1, ..., \nabla f_n$. The random variable $X$ is said to be in $L_1$ (respectively, $L_2$) if $E[|X|] < +\infty$ (resp., $E[X^2] < +\infty$). For two symmetric matrices $A, B$ of the same size, we write $A \preceq B$ if and only if $B - A$ is positive semi-definite.

2. Mathematical results

2.1. A Second Order Stein formula

Stein’s formula (1.1) states that the random variable

$$(2.1) \quad z^\top f(z) - \text{div} f(z)$$

is mean-zero. The main result of the current paper is the following Second Order Stein formula, which provides an identity for the variance of the random variable (2.1) with $f$ in the Sobolev space $W^{1,2}(\gamma_n)$ with respect to the standard Gaussian measure $\gamma_n$ in $\mathbb{R}^n$. Let $C^\infty_0(\mathbb{R}^n)$ be the space of infinitely differentiable functions $\mathbb{R}^n \to \mathbb{R}$ with compact support. The Sobolev space $W^{1,2}(\gamma_n)$ is defined as the completion of the space $C^\infty_0(\mathbb{R}^n)$ with respect to the norm

$$(2.2) \quad \|g\|_{1,2} = E[g(z)^2]^{1/2} + E[\|\nabla g(z)\|^2]^{1/2}, \quad g \in C^\infty_0(\mathbb{R}^n)$$

where $z \sim N(0, I_n)$. By [Bog98, Proposition 1.5.2], the space $W^{1,2}(\gamma_n)$ corresponds to locally integrable functions $g : \mathbb{R}^n \to \mathbb{R}$ that are weakly differentiable and $E[g(z)^2] + E[\|\nabla g(z)\|^2] < +\infty$ for $z \sim N(0, I_n)$. This definition of the Sobolev space emphasizes the feasibility of approximating the functions in the space by infinitely smooth ones. Alternatively, $W^{1,2}(\gamma_n)$ can be defined as the completion of the space of Lipschitz functions under the same norm. We refer to Section 1.5 in [Bog98] for a complete description of the space $W^{1,2}(\gamma_n)$. 
Theorem 2.1. Let $z = (z_1, ..., z_n)$ be a standard normal $N(0, I_n)$ random vector. Let $f_1, ..., f_n$ be functions $\mathbb{R}^n \to \mathbb{R}$ and $f$ be the column vector in $\mathbb{R}^n$ with $i$-th component equal to $f_i$. Assume throughout that each $f_i$ is square integrable, i.e. $\mathbb{E}[f_i(z)^2] < \infty$.

(i) Assume that each $f_i$ is twice continuously differentiable and that its first and second order derivatives have sub-exponential growth. Then

$$
\mathbb{E} \left[(z^T f(z) - \text{div} f(z))^2\right] = \mathbb{E} \sum_{i=1}^n f_i^2(z) + \mathbb{E} \sum_{i=1}^n \sum_{j=1}^n \frac{\partial f_i}{\partial x_j}(z) \frac{\partial f_j}{\partial x_i}(z).
$$

An equivalent version of (2.3) for functions of $y = N(\mu, \sigma^2 I)$, in vector notation, is given in (2.7) below.

(ii) If $f : \mathbb{R}^n \to \mathbb{R}^n$ is $L$-Lipschitz for $L < +\infty$, then (2.3) holds.

(iii) If each component $f_i$ of $f$ belongs to $W^{1,2}(\gamma_n)$, then (2.3) holds.

We note that while (i) and (ii) may have broader appeal due to their simplicity, the assumption in (iii) above is the most general: If $f$ satisfies either the assumption in (i) or (ii) then the components of $f$ are in $W^{1,2}(\gamma_n)$ and the assumption in (iii) holds. The presentation above also highlights the proof strategy: We first derive (2.3) under the smoothness assumption in (i) and (ii)-(iii) then follow by an approximation argument.

Here is a proof of Theorem 2.1(i). Extensions (ii) and (iii) are proved in Appendix A.

Proof of Theorem 2.1 (i). When the functions $f_i$ and $(\partial/\partial x_j)f_i$ are treated as random variables, their argument is always $z$ through the proof, so we simply write $f_i$ for $f_i(z)$ and similarly for the partial derivatives. A sum $\sum_i$ or $\sum_k$ always sums over $\{1, ..., n\}$.

Write the left hand side in (2.3) as

$$
\mathbb{E} \sum_i \left(z_i f_i - \frac{\partial f_i}{\partial x_i} \right) \left( \sum_j z_j f_j - \sum_l \frac{\partial f_l}{\partial x_l} \right).
$$

By a first application of Stein’s formula for each term $z_i$ below, the identity

$$
\mathbb{E} \left[(z_i f_i(z) - \frac{\partial f_i}{\partial x_i}(z)) g(z)\right] = \mathbb{E} \left[f_i(z) \frac{\partial g}{\partial x_i}(z)\right]
$$

holds for any continuously differentiable function $g : \mathbb{R}^n \to \mathbb{R}$ such that the partial derivatives $(\partial/\partial x_i)g$ have sub-exponential growth. Hence the left hand side in (2.3) equals

$$
\mathbb{E} \sum_i f_i^2 + \mathbb{E} \sum_i f_i \sum_j z_j \frac{\partial f_j}{\partial x_i} - \mathbb{E} \sum_i f_i \sum_l \frac{\partial^2 f_l}{\partial x_i \partial x_l}.
$$

We again apply Stein’s formula to each $z_j$ in the second term above to obtain

$$
\mathbb{E} \sum_i f_i^2 + \mathbb{E} \sum_i \sum_j \frac{\partial f_i}{\partial x_j} \frac{\partial f_j}{\partial x_i} + \mathbb{E} \sum_i f_i \sum_j \frac{\partial^2 f_j}{\partial x_j \partial x_i} - \mathbb{E} \sum_i f_i \sum_l \frac{\partial^2 f_l}{\partial x_i \partial x_l}.
$$
Since $f$ is twice continuously differentiable, by the Schwarz theorem on the symmetry of the second derivatives we have $\sum_j (\partial/\partial x_j)(\partial/\partial x_i)f_j = \sum_i (\partial/\partial x_i)(\partial/\partial x_j)f_i$ and the proof of (2.3) is complete. $\Box$

The Second Order Stein formula (2.3) can then be rewritten as

\begin{equation}
E[(z^TF(z) - \text{div} f(z))^2] = E[\|f(z)\|^2 + \text{trace}((\nabla f(z))^2)].
\end{equation}

By the Cauchy-Schwarz inequality,

\begin{equation}
E[(z^TF(z) - \text{div} f(z))^2] \leq E\sum_{i=1}^n f_i^2(z) + E\sum_{i=1}^n \sum_{j=1}^n \left(\frac{\partial f_i}{\partial x_j}(z)\right)^2,
\end{equation}

If $\nabla f(z)$ is almost surely symmetric, then $\text{trace}((\nabla f(z))^2) = \|\nabla f(z)\|^2_F$ and the above inequality is actually an equality. However the inequality in (2.6) is strict otherwise.

If $y = \mu + \varepsilon$ with $\varepsilon \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_n)$ and $f : \mathbb{R}^n \to \mathbb{R}^n$ then

\begin{equation}
E[(\varepsilon^T f(y) - \sigma^2 \text{div} f(y))^2] = \sigma^2 E[\|f(y)\|^2] + \sigma^4 E[\text{trace}((\nabla f(y))^2)]
\end{equation}

is obtained by setting $z = \varepsilon/\sigma$ and applying Theorem 2.1 to $\tilde{f}(x) = \sigma f(\mu + \sigma x)$, provided that $\tilde{f}$ satisfies the assumption of Theorem 2.1 (iii). Similarly if $y = \mu + \varepsilon$ with $\varepsilon \sim N(\mathbf{0}, \Sigma)$ then

\begin{equation}
E[(\varepsilon^T f(y) - \text{trace}(\Sigma \nabla f(y)))^2] = E[\|\Sigma^{1/2} f(y)\|^2] + \text{trace}\left[\left(\Sigma \nabla f(y)\right)^2\right]
\end{equation}

follows from Theorem 2.1 with $z = \Sigma^{-1/2} \varepsilon$ and $\tilde{f}(x) = \Sigma^{1/2} f(\mu + \Sigma^{1/2} x)$.

Theorem 2.1 is also applicable under the central limit theorem. Let $\varepsilon_m = m^{-1/2} \sum_{i=1}^m x_i$ with $\text{id} x_i \in \mathbb{R}^n$, $E[x_i] = \mathbf{0}$ and $E[x_i x_j^T] = \Sigma$. If $\|f(\varepsilon_m)\|^2, \|\nabla f(\varepsilon_m)\|^2_F, (\varepsilon_m^T f(\varepsilon_m))^2, m \geq 1$ is uniformly integrable and $\nabla f$ is almost everywhere continuous, then $E[\varepsilon_m^T f(\varepsilon_m)] = E[\text{trace}(\Sigma \nabla f(\varepsilon_m))] + o(1)$ and

\begin{equation}
E\left[\left(\varepsilon_m^T f(\varepsilon_m) - \text{trace}(\Sigma \nabla f(\varepsilon_m))\right)^2\right] \leq E[\|\Sigma^{1/2} f(\varepsilon_m)\|^2] + \text{trace}\left[\left(\Sigma \nabla f(\varepsilon_m)\right)^2\right] + o(1)
\end{equation}

as $m \to \infty$ for fixed $n$. If, for instance, $f : \mathbb{R}^n \to \mathbb{R}^n$ is $L$-Lipschitz with almost everywhere continuous gradient and $E[\|x\|^4] \leq C$ for some constant $C > 0$ possibly depending on the dimension, then $\{\|\varepsilon_m\|^4, m \geq 1\}$ is uniformly integrable, which implies that $\{\|f(\varepsilon_m)\|^2, \|\nabla f(\varepsilon_m)\|^2_F, (\varepsilon_m^T f(\varepsilon_m))^2, m \geq 1\}$ is also uniformly integrable, so that (2.8) holds by, e.g., [VDW96, Theorem 1.11.3].
2.2. **Inner-product structure**

The two sides of (2.5) are quadratic in \( f \) and (2.5) is endowed with an inner-product structure. Indeed, if \( f, h : \mathbb{R}^n \to \mathbb{R}^n \) satisfy the assumption of Theorem 2.1(iii), so do \( f + h \) and \( f - h \). Applying (2.5) to \( f + h \) and \( f - h \), taking the difference and dividing by 4 yield

\[
\mathbb{E} \left[ \{ z^\top f(z) - \text{div} f(z) \} \{ z^\top h(z) - \text{div} h(z) \} \right] = \mathbb{E} \left[ f(z)^\top h(z) + \text{trace} (\nabla f(z)\nabla h(z)) \right]
\]

(2.9)

thanks to \( \text{trace} (\nabla f(z)\nabla h(z)) = \text{trace} (\nabla h(z)\nabla f(z)) \).

2.3. **Extensions and upper bounds on variance**

The Second Order Stein formula (2.3) lets us derive the variance of more general random variables of the form

\[
z^\top f(z) - \sigma^2 \text{div} f(z) - g(z)
\]

(2.10)

and a related upper bound for the variance, where \( z \sim N(0, \sigma^2 I_n) \) and \( f : \mathbb{R}^n \to \mathbb{R}^n \) and \( g : \mathbb{R}^n \to \mathbb{R} \) satisfy the smoothness and integrability conditions of respective dimensions as in Theorem 2.1. The formula for the variance of (2.10) can be viewed as an extension of (2.3) from \( g = 0 \) to general \( g \). As a special case, this provides a formula and an upper bound for the variance of the divergence with \( g(x) = x^\top f(x) \).

**Theorem 2.2.** Let \( z \sim N(0, \sigma^2 I_n) \), \( f \) be as in Theorem 2.1 and \( g \in W^{1,2}(\gamma_n) \). Then the variance of the random variable in (2.10) satisfies

\[
\text{Var}(z^\top f(z) - \sigma^2 \text{div} f(z) - g(z)) = \mathbb{E} \left[ \sigma^2 \| f(z) - \nabla g(z) \|^2 + \sigma^4 \text{trace} (\nabla f(z)^2) \right] + \tilde{V}(g)
\]

(2.11)

\[
\leq \mathbb{E} \left[ \sigma^2 \| f(z) - \nabla g(z) \|^2 + \sigma^4 \text{trace} (\nabla f(z)^2) \right].
\]

(2.12)

with \( \tilde{V}(g) = \text{Var}(g(z)) - \sigma^2 \mathbb{E}[\| \nabla g(z) \|^2] \). In particular, with \( g(x) = x^\top f(x) \),

\[
\text{Var} [\text{div} f(z)] = \mathbb{E} [\text{trace} (\nabla f(z)^2)] + \text{Var} [z^\top f(z)/\sigma^2] - \mathbb{E}[\| f(z)/\sigma \|^2] - 2 \mathbb{E}[z^\top (\nabla f(z))z/\sigma^2]
\]

(2.13)

\[
\leq \mathbb{E} [\text{trace} (\nabla f(z)^2)] + \mathbb{E}[\| \nabla f(z)z/\sigma \|^2].
\]

**Proof.** Assume without loss of generality \( \sigma = 1 \). By (2.4),

\[
\mathbb{E} \left[ (z^\top f(z) - \text{div} f(z)) g(z) \right] = \mathbb{E} \left[ f(z)^\top \nabla g(z) \right],
\]

so that (2.11) follows from Theorem 2.1 and some algebra. The Gaussian Poincaré inequality [BLM13, 3.20] applied to \( g \) reads \( \tilde{V}(g) \leq 0 \) which gives (2.12). Finally, for \( g(x) = x^\top f(x) \), we have \( (\partial g/\partial x)(z) = f_i(z) + \sum_{j=1}^n z_j (\partial f_j/\partial x_i)(z) \) so that \( \nabla g(z) = f(z) + (\nabla f(z))z \). \( \square \)
As we have mentioned earlier, (2.11) becomes (2.7) when \( g = 0 \). The extension in Theorem 2.2 is particularly useful in our investigation of the variance of SURE and other quantities of interest. A striking feature of the upper bound in (2.13) is that the variance of the random variable \( \text{div} f(z) \), defined using the first order derivatives of \( f \), can be bounded from above using only the first order partial derivatives of \( f \). In particular, the second partial derivatives of \( f \) may be arbitrarily large or may not exist. This feature will be used in the next section to study the variance of the size of the model selected by the Lasso in linear regression, which takes the form \( \text{div} f \) for a certain function \( f \).

It can be seen from the definition of \( V(g) \) that the inequality (2.12) involves a single application of the Gaussian Poincaré inequality to \( g(z) \). Thus, it holds with equality if and only if \( g(x) \) is linear.

Finally, we obtain the following by applying Theorem 2.2 to \( g(x) = x^\top \{ f(x) - \mathbb{E}[\nabla f(z)]x \} \):

\[
(2.14) \quad \text{Var}[\text{div} f(z)] \\
\leq \mathbb{E}[\text{trace} (\{ \nabla f(z) - \mathbb{E}[\nabla f(z)] \})^2] + \mathbb{E}[\| \{ \nabla f(z) - \mathbb{E}[\nabla f(z)] \} z/\sigma \|^2].
\]

This recovers \( \text{Var}[\text{div} f(z)] = 0 \) when \( f(z) \) is linear in \( z \) and may be useful in other cases where \( \nabla f(z) - \mathbb{E}[\nabla f(z)] \) is small.

### 2.4. Beyond Gaussian distributions

Although the next section provides applications of (2.5) and (2.12) in the Gaussian case only, we briefly mention here extensions to non-Gaussian \( z \) when \( z \) has density \( x \to \exp(-\psi(x)) \) where \( \psi : \mathbb{R}^n \to \mathbb{R} \) is twice continuously differentiable with Hessian \( H(x) = \nabla^2 \psi(x) \). Throughout, let \( h, f : \mathbb{R}^n \to \mathbb{R}^n \) be smooth vector fields with compact support and \( g : \mathbb{R}^n \to \mathbb{R} \) be smooth. By integration by parts,

\[
\int \{ \nabla \psi(z)^\top h(z) - \text{div} h(z) \} g(z)e^{-\psi(z)} \, dz = \int h(z)^\top \nabla g(z)e^{-\psi(z)} \, dz.
\]

Applying this identity twice, first to \( h = f \) and \( g(x) = \nabla \psi(x)^\top f(x) - \text{div} f(x) \), second to \( h(x) = \nabla f(x)^\top f(z) \) and \( g = 1 \) gives

\[
(2.15) \quad \mathbb{E}[\{ \nabla \psi(z)^\top f(z) - \text{div} f(z) \}^2] = \mathbb{E}[\{ f(z)^\top (H(z)) f(z) + \text{trace} (\nabla f(z)^2) \}]
\]

which extends (2.3) to non-Gaussian distributions. Similarly to Theorem 2.2, if \( \psi \) is additionally strictly convex then

\[
(2.16) \quad \text{Var}(\nabla \psi(z)^\top f(z) - \text{div} f(z) - g(z)) = \mathbb{E}[\| H(z)^{1/2} f(z) - H(z)^{-1/2} \nabla g(z) \|^2 + \text{trace} (\{ \nabla f(z) \}^2)] + \tilde{V}(g)
\]

where \( \tilde{V}(g) = \text{Var}(g(z)) - \mathbb{E}[\| H(z)^{1/2} \nabla g(z) \|^2] \) and \( \tilde{V}(g) \leq 0 \) follows from the Brascamp-Lieb inequality [BGL13, Theorem 4.9.1]. In the special case where
f = ∇u for some smooth u : ℝⁿ → ℝ, identity (2.15) is related to the Bochner formula used in the analysis of diffusion operators [BGL13, Section 1.16.1], which gives hope to extend (2.3) and its applications to probability measures defined on non-Euclidean manifolds—although this goal lies outside of the scope of the present paper.

3. Statistical applications

3.1. SURE for SURE

In the Gaussian sequence model, one observes \( y = \mu + \varepsilon \) where the noise \( \varepsilon \sim N(0, I_n) \) is standard normal and \( \mu \) is an unknown mean. Given an estimator \( \hat{\mu}(y) \) where \( \hat{\mu} : ℝ^n → ℝ^n \) is some known almost differentiable function with \( \nabla \hat{\mu}(y) \) in \( L_1 \), SURE provides an unbiased estimate of the mean squared risk \( E\|\hat{\mu} - \mu\|^2 \) given by

\[
\hat{\text{SURE}} = \|\hat{\mu} - y\|^2 + 2 \text{div} \hat{\mu}(y) - n.
\]

(3.1)

The fact that this quantity is an unbiased estimate of \( E\|\hat{\mu} - \mu\|^2 \) is a consequence of the identity

\[
\|\hat{\mu} - \mu\|^2 = \|\hat{\mu} - y\|^2 + 2 \varepsilon^\top (\hat{\mu} - \mu) - \|\varepsilon\|^2
\]

with \( E[\|\varepsilon\|^2] = n \) and Stein’s formula (1.1) which asserts that \( E[\varepsilon^\top \hat{\mu}(y)] = E[\text{div} \hat{\mu}(y)] \) whenever all partial derivatives of \( \hat{\mu} \) are in \( L_1 \). The random variable \( \text{div} \hat{\mu}(y) \) can be computed from the observed data since it only involves \( y \) as well as the partial derivatives of \( \hat{\mu} \). The quantity \( \hat{df} = \text{div} \hat{\mu}(y) \) is an estimator sometimes referred to as the empirical degrees of freedom of the estimator \( \hat{\mu} \).

In this subsection, we develop Second Order Stein methods to evaluate the accuracy of SURE.

3.1.1. SURE for SURE in general

We define the mean squared risk of the scalar estimator \( \hat{\text{SURE}} \) by

\[
R_{\text{SURE}} = E\left[ \left( \hat{\text{SURE}} - \|\hat{\mu} - \mu\|^2 \right)^2 \right].
\]

(3.2)

This means we treat \( \hat{\text{SURE}} \) as an estimate of the squared prediction error \( \|\hat{\mu} - \mu\|^2 \) as well. This is reasonable as the actual squared loss \( \|\hat{\mu} - \mu\|^2 \) is often a more relevant target than its expectation. One may also wish to treat \( \hat{\text{SURE}} \) as an estimate of the deterministic \( E[\|\hat{\mu} - \mu\|^2] \) and consider the estimation of \( \text{Var}(\hat{\text{SURE}}) \). Thanks to Theorem 2.2, we will develop in the next subsection methodologies for the consistent estimation of upper bounds for \( \text{Var}(\hat{\text{SURE}}) \) and \( R_{\text{SURE}} \) under proper conditions on the gradient of \( \hat{\mu} \).

SURE is widely used in practice to estimate \( \|\hat{\mu} - \mu\|^2 \) or \( E[\|\hat{\mu} - \mu\|^2] \) either because it is of interest to estimate the prediction error of \( \hat{\mu} \), or because several...
estimators of the mean vector $\mu$ are available and the statistician hopes to use the $\hat{\text{SURE}}$ to compare them on equal footing. Although $\hat{\text{SURE}}$ provides an unbiased estimate of the loss $\|\hat{\mu} - \mu\|^2$ and its expectation, such estimate may end up being not so useful, or provide spurious estimates, if the quantity (3.2) is too large. For estimators of interest where $\hat{\text{SURE}}$ is used in practice, it is important to understand the risk of $\hat{\text{SURE}}$ given by (3.2) in order to provide some uncertainty quantification about the accuracy of $\hat{\text{SURE}}$. For instance, one should expect $\hat{\text{SURE}}$ to be successful if $R_{\text{SURE}}^{1/2}$ is negligible compared to $\hat{\text{SURE}}$, i.e., $R_{\text{SURE}}^{1/2} \ll \hat{\text{SURE}}$. On the other hand, if $R_{\text{SURE}}^{1/2} \gg \hat{\text{SURE}}$ then we would expect that estimates from $\hat{\text{SURE}}$ would be spurious with strictly positive probability and $\hat{\text{SURE}}$ should not be trusted. Under the square integrability condition on the first and second partial derivatives of $f(y)$, [Ste81] proposed an unbiased estimate of the risk (3.2). However, the twice differentiability condition typically fails to hold for estimators involving less smooth regularizers such as the Lasso. [DJ95] studied the performance of SURE optimized separable threshold estimator (SureShrink) and thus the accuracy of SURE in this special case. [DKF+13] derives an identity for the quantity (3.2) in the special case of the Lasso. In a general study of SURE tuned estimators, [TR18] developed a correction for the excess optimism with the nominal SURE in such schemes. Section 5 in [JM18] establishes consistency of SURE for the Lasso when the design matrix has iid $N(0, 1)$ entries and the tuning parameter is large enough. The Second Order Stein identity

$$E\left[\left\{\|z\|^2 - n + \gamma(z)\right\}^2\right] = E\left[2p + 2\Delta \gamma(z) + \gamma(z)^2\right],$$

where $\Delta = \sum_{i=1}^n (\partial/\partial x_i)^2$ is the Laplacian, was used in [Joh88] to prove the inadmissibility of SURE for the estimation of the squared loss of the James-Stein estimator when $n \geq 5$.

The following result, which extends Theorem 3 of [Ste81] to allow application to the Lasso and other estimators only one-time differentiable, computes the expectation of the quantity (3.2) as well as an unbiased estimator of it directly through Theorem 2.1.

**Theorem 3.1.** Let $\varepsilon \sim N(0, I_n)$ and $y = \mu + \varepsilon$. Let $\hat{\mu}$ be an estimator of $\mu$ with $\hat{\mu} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ satisfying the assumptions of Theorem 2.1, and define $\hat{\text{SURE}}$ by (3.1). Then

$$E\left[\left(\text{SURE} - \|\hat{\mu} - \mu\|^2\right)^2\right] = E\left[4\|y - \hat{\mu}(y)\|^2 + 4 \text{trace}((\nabla \hat{\mu}(y))^2) - 2n\right].$$

Consequently, SURE for SURE

$$\hat{R}_{\text{SURE}} = 4\|y - \hat{\mu}(y)\|^2 + 4 \text{trace}((\nabla \hat{\mu}(y))^2) - 2n$$

is an unbiased estimate of the risk of $\hat{\text{SURE}}$ in (3.2).

**Remark 3.1.** With the notation $f(y) = \hat{\mu} - y$ used in [Ste81], $\nabla f(y) = \nabla \hat{\mu}(y) - I_n$ and SURE for SURE is also given by

$$\hat{R}_{\text{SURE}} = 2n + 4\|f(y)\|^2 + 4 \text{trace}((\nabla f(y))^2) + 8 \text{div} f(y).$$
Proof. Write $\text{div} \hat{\mu}$ for $\text{div} \hat{\mu}(y)$ and $\hat{\mu}$ for $\hat{\mu}(y)$. By simple algebra

$$(\|\hat{\mu} - \mu\|^2 - \text{SURE})^2 = (\varepsilon^T \{2(\hat{\mu} - y) + \varepsilon\} + (n - 2 \text{div} \hat{\mu}))^2.$$ 

By (2.7) applied to $y \to 2\{\hat{\mu}(y) - y\} + (y - \mu)$ we obtain in expectation

$$R_{\text{SURE}} = \mathbb{E}[\|2\{\hat{\mu} - y\} + \varepsilon\|^2 + \text{trace}\{(2\nabla \hat{\mu} - I_n)^2\}]$$  

$$= \mathbb{E}[4\|\hat{\mu} - y\|^2 + 4\text{trace}\{(\nabla \hat{\mu})^2\} - 2n]$$  

$$+ \mathbb{E}[4\varepsilon^T(\hat{\mu} - y) + 4(n - \text{div} \hat{\mu})].$$  

The proof of (3.3) is complete as the last line is 0 in virtue of Stein’s formula.

Equality (3.5) is obtained by observing that $f(y) = \hat{\mu}(y) - y$, hence

$$\nabla f(y) = \nabla \hat{\mu} - I_n, \quad \text{div} f(y) = \text{trace}[\nabla \hat{\mu}] - n,$$

$$4\text{trace}[(\nabla f(y))^2] + 8\text{div} f(y) = 4\text{trace}[(\nabla \hat{\mu}(y))^2] - 4n.$$

Remark 3.2. In the Gaussian sequence model where the noise $\varepsilon$ has distribution $N(0, \sigma^2 I_n)$ with $\sigma \neq 1$, the estimator $\text{SURE}$ has the form

$$(3.7) \quad \text{SURE} = \|y - \hat{\mu}\|^2 + 2\sigma^2 \text{div} \hat{\mu} - \sigma^2 n.$$

Theorem 3.1 implies that in this setting, SURE for SURE is

$$(3.8) \quad \hat{R}_{\text{SURE}} = 4\sigma^2 \|y - \hat{\mu}\|^2 + 4\sigma^4 \text{trace}[(\nabla \hat{\mu})^2] - 2\sigma^4 n,$$

as its expectation is identical to $R_{\text{SURE}} = \mathbb{E}[(\text{SURE} - \|\hat{\mu} - \mu\|^2)^2]$.

3.1.2. Error bounds and consistency

In the spirit of SURE, SURE for SURE in (3.8) is fundamentally a point estimator for the risk of SURE as defined in (3.2). It could be the starting point for the construction of an interval estimator or simply provide some measure of the performance of SURE when nothing else or better is available. Because of its availability in broad settings, (3.8) is not expected to always yield sensible and theoretically justifiable interval estimates. Still, we provide here consistent estimation of upper bounds for both the risk (3.2) and $\text{Var}(\text{SURE})$ under proper conditions on $\hat{\mu}$. Furthermore, when the gradient is a random orthogonal projection as in Lasso, isotonic regression and many other cases, the theorem below proves the consistency of SURE for SURE in (3.8). Define

$$(3.9) \quad \hat{R}'_{\text{SURE}} = 2\sigma^2 (\|y - \hat{\mu}\|^2 + \text{SURE}),$$

which satisfies $\hat{R}'_{\text{SURE}} - \hat{R}_{\text{SURE}} = 4\sigma^4 \{\text{div} \hat{\mu} - \text{trace}[(\nabla \hat{\mu})^2]\}$ compared with SURE for SURE in (3.8). In particular, $\hat{R}'_{\text{SURE}} = \hat{R}_{\text{SURE}}$ if $\nabla \hat{\mu}$ is a random orthogonal projection.
**Theorem 3.2.** Let \( \widehat{\text{SURE}} \), \( \widehat{R}_{\text{sparse}} \), \( \widehat{\mu} \), and \( \widehat{R}'_{\text{sparse}} \) be as in (3.7), (3.2), (3.8) and (3.9) respectively and assume \( y = \mu + \varepsilon \) with \( \varepsilon \sim N(0, \sigma^2 I_n) \).

(i) If \( E \sum_{i=1}^n |(\nabla \widehat{\mu})_i| < +\infty \), then \( E[\widehat{R}'_{\text{sparse}}] \geq \sigma^4 n \).

(ii) If the function \( y \rightarrow \widehat{\mu}(y) \) is 1-Lipschitz, then

\[
E \left[ \left( (\widehat{\text{SURE}})_{+}^{1/2} - E[\|\widehat{\mu} - \mu\|]^{1/2} \right)^4 \right]^{1/4} \leq \frac{R_{\text{sparse}}}{n} + 3\sigma.
\]

(iii) If the function \( y \rightarrow \widehat{\mu}(y) \) is 1-Lipschitz and \( \nabla \widehat{\mu} \) is almost everywhere symmetric positive semi-definite, then \( \widehat{R}_{\text{sparse}} \leq \widehat{R}'_{\text{sparse}} \) and

\[
\text{Var}(\widehat{\text{SURE}}) = \frac{1}{E}[\widehat{R}'_{\text{sparse}} - 1] \leq \frac{16\sigma^4}{E[\widehat{R}'_{\text{sparse}}]} \leq \frac{16\sigma^4}{n}
\]

**Remark 3.3.** If \( \widehat{\mu}(y) = X\beta(y) \) for some fixed \( X \in \mathbb{R}^{n \times p} \) and a penalized estimator \( \beta(y) = \arg \min_{b \in \mathbb{R}^p} \{ \| y - Xb\|^2 + g(b) \} \) for convex \( g : \mathbb{R}^p \rightarrow \mathbb{R} \), then \( \widehat{\mu} \) is 1-Lipschitz and \( \nabla \widehat{\mu}(y) \) is almost everywhere symmetric positive semi-definite. This follows from arguments in [BT17, BZ19] as explained at the end of Appendix B. Hence for any convex regularized least-squares estimate \( \beta(y) \), \( \widehat{\mu}(y) = X\beta(y) \) satisfies the conditions in (ii)-(iv) above as well as \( \widehat{R}_{\text{sparse}} \leq \widehat{R}'_{\text{sparse}} \) almost surely.

If the estimation of the deterministic quantity \( E[\|\widehat{\mu} - \mu\|^2] \) is essential, inequality (3.10) asserts that up to an additive absolute constant, \( R_{\text{sparse}} \) bounds from above the quartic risk of \( \widehat{\text{SURE}}^{1/2} \) when the estimation target is \( E[\|\widehat{\mu} - \mu\|^2]^{1/2} \). If in addition the gradient is almost everywhere symmetric positive semi-definite as in Remark 3.3, inequality (3.11) asserts that the risk \( \text{Var}(\widehat{\text{SURE}}) \) is bounded from above by \( R_{\text{sparse}} + \sigma^4 n \leq 2E[\widehat{R}'_{\text{sparse}}] \), with a slight modification \( \widehat{R}'_{\text{sparse}} \) of the SURE for SURE. Moreover, under milder conditions in Theorem 3.2 (iv) which do not require the symmetry of the random matrix \( \nabla \widehat{\mu} \), \( \widehat{R}'_{\text{sparse}} \) is a consistent estimator of its expectation.

When the gradient \( \nabla \widehat{\mu} \) is a random orthogonal projection, \( \widehat{R}'_{\text{sparse}} \) is identical to \( \widehat{R}_{\text{sparse}} \), so that SURE for SURE is a consistent estimator of its risk \( R_{\text{sparse}} \) and \( R_{\text{sparse}} + \sigma^4 n \leq 2R_{\text{sparse}} \) are upper bounds for the risk \( \text{Var}(\widehat{\text{SURE}}) \). In the lasso case, \( \nabla \widehat{\mu} \) is an orthogonal projection, cf. Section 3.5.1 below.

The proof of Theorem 3.2 is given in Appendix B. In fact, under the conditions for (3.12), we prove the sharper

\[
\text{Var}(\widehat{R}'_{\text{sparse}}) \leq 16\sigma^4 E[\widehat{R}'_{\text{sparse}}^2]
\]

with \( \widehat{R}_{\text{sparse}}'' = (3/4)\widehat{R}'_{\text{sparse}} + (1/4)\widehat{R}_{\text{sparse}} - \sigma^4 \text{div} \widehat{\mu} \leq \widehat{R}'_{\text{sparse}} \). This suggests the use of \( 16\sigma^4 \widehat{R}_{\text{sparse}}'' \) or \( 16\sigma^4 \widehat{R}'_{\text{sparse}} \) as estimated upper bounds for \( \text{Var}(\widehat{R}_{\text{sparse}}) \).
3.1.3. Difference of two estimators

As we have briefly discussed above the statement of Theorem 3.1, SURE is often used to optimize among different estimators. Consider for simplicity the comparison between two estimates \( \hat{\mu}^{(1)} \) and \( \hat{\mu}^{(2)} \) of \( \mu \). In this setting, \( R_{\text{sure}}^{(\text{diff})} = E \left[ \left( \| \hat{\mu}^{(1)} - \mu \|^2 - \| \hat{\mu}^{(2)} - \mu \|^2 - \hat{\text{SURE}}^{(\text{diff})} \right)^2 \right] \) is the proper risk for SURE, where \( \hat{\text{SURE}}^{(\text{diff})} = \hat{\text{SURE}}^{(1)} - \hat{\text{SURE}}^{(2)} = \| \hat{\mu}^{(1)} - y \|^2 - \| \hat{\mu}^{(2)} - y \|^2 + 2 \text{div} (\hat{\mu}^{(1)} - \hat{\mu}^{(2)}) \) is the difference in SURE between \( \hat{\mu}^{(1)} \) and \( \hat{\mu}^{(2)} \). When the loss \( \| \hat{\mu} - \mu \|^2 \) is of smaller order than \( n^{1/2} \), SURE may produce a spurious estimator due to the estimation of \( \| \epsilon \|^2 \) by \( n \) in (3.1). However, due to the cancellation of this common chi-square type error, the risk of the estimator (3.15) could be of smaller order than the risk of SURE for both \( \hat{\mu}^{(j)} \). Parallel to Theorem 3.1, the Second Order Stein formula leads to the following.

**Theorem 3.3.** Let \( \epsilon \sim N(0, I_n) \), \( y = \mu + \epsilon \), and \( \hat{\mu}^{(1)} \) and \( \hat{\mu}^{(2)} \) be estimates of \( \mu \) based on \( y \). Let \( \hat{\text{SURE}}^{(\text{adj})} \) and \( R_{\text{sure}}^{(\text{adj})} \) be as in (3.15) and (3.14) respectively and \( f(y) = \hat{\mu}^{(1)} - \hat{\mu}^{(2)} \). Suppose \( f : \mathbb{R}^n \to \mathbb{R}^n \) satisfies the assumptions of Theorem 2.1. Then, 

\[
R_{\text{sure}}^{(\text{adj})} = E \left[ 4\| f(y) \|^2 + 4 \text{trace} \left( (\nabla f(y))^2 \right) \right].
\]

Consequently, SURE for SURE, given by 

\[
\hat{R}_{\text{sure}}^{(\text{adj})} = 4\| f(y) \|^2 + 4 \text{trace} \left( (\nabla f(y))^2 \right),
\]

is an unbiased estimate of the risk of \( \hat{\text{SURE}}^{(\text{adj})} \) in (3.14).

**Proof.** By algebra, 

\[
\| \hat{\mu}^{(1)} - \mu \|^2 - \| \hat{\mu}^{(2)} - \mu \|^2 - \hat{\text{SURE}}^{(\text{diff})} = 2\epsilon^\top f(y) - 2 \text{div} f(y).
\]

The conclusion follows directly from Theorem 2.1.

3.2. Confidence region based on \( \text{SURE} \)

While SURE for SURE provides an unbiased point estimator for the (mean) squared difference between \( \text{SURE} \) and the squared loss \( \| \hat{\mu} - \mu \|^2 \), we may also use the Second Order Stein formula to derive interval estimates for \( \| \hat{\mu} - \mu \|^2 \) and \( E[\| \hat{\mu} - \mu \|^2] \) based on \( \text{SURE} \). As we are not compelled to directly use the \( \hat{R}_{\text{sure}} \) in (3.8) to construct such interval estimates, we present the following simpler approach.
Theorem 3.4. Let $\mathbf{y}, \mu, \hat{\mu} = \hat{\mu}(\mathbf{y})$ and $\text{SURE}$ be as in (3.7). Then,

$$E\left[ (\text{SURE} - ||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2 - ||\varepsilon||^2 + \sigma^2 n)^2 \right] = 4\sigma^2 E[||\hat{\mathbf{\mu}} - \mathbf{\mu}||^2] + 4\sigma^4 E[\text{trace}(\nabla \hat{\mathbf{\mu}}^2)].$$

If the right-hand side of (3.18) is bounded by $\sigma^4 v_0^2 2n\epsilon_n$ with a constant $v_0$, then

$$P\left\{ ||\text{SURE} - ||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2| \leq \sigma^2 (v_0 + \epsilon_n)\sqrt{n} \right\} \geq 1 - \alpha - \epsilon_n$$

for all $\alpha \in (0, 1)$, where $v_\alpha$ is defined by $P\{(2n)^{-1/2}|\chi_n^2 - n| > v_\alpha\} = \alpha$, and

$$P\left\{ ||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2 \leq \text{SURE} + \sigma^2 (v_{-\alpha} + \epsilon_n)\sqrt{n} \right\} \geq 1 - \alpha - \epsilon_n,$$

where $v_{-\alpha}$ is defined by $P\{(2n)^{-1/2}(n - \chi_n^2) > v_{-\alpha}\} = \alpha$.

While the left-hand side of (3.18) is quartic in $||\hat{\mathbf{\mu}} - \mathbf{\mu}||$, the right-hand side is quadratic. Thus, $\text{SURE}$ provides an accurate estimate of $||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2$ when the squared error is of greater order than $||\varepsilon||^2 - \sigma^2 n) \approx \sigma^2 (2n)^2 N(0, 1)$, provided that the second term on the right-hand side of (3.18) is of no greater order than $\max \{ \sigma^4 n, \sigma^2 E[||\hat{\mathbf{\mu}} - \mathbf{\mu}||^2] \}$. Specifically, in such scenarios, (3.19) implies that $\text{SURE}$ is within a small fraction of $||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2$ when $\sqrt{||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2/n}$ is of greater order than $\sigma n^{-1/4}$, and (3.19) and (3.20) provide confidence regions for the entire vector $\mathbf{\mu}$. As $\sigma n^{-1/4}$ is known to be a lower bound for the error in the estimation of the average loss in the estimation of $\mathbf{\mu}$ [Li89, NvdG13], (3.19) implies the rate optimality of the upper bound (3.20) for the squared estimation error $||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2$ and thus the rate optimality of the resulting confidence region for $\mathbf{\mu}$.

Corollary 3.5. If for some sequence $(\gamma_n)$ with $\gamma_n \to 0$

$$E[4||\hat{\mathbf{\mu}} - \mathbf{\mu}||^2/(n\sigma^2) + 4\text{trace}(\nabla \hat{\mathbf{\mu}}^2)/n] \leq \gamma_n,$$

then for all fixed $\alpha \in (0, 1)$ independent of $n$,

$$P\left\{ ||\text{SURE} - ||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2| \leq \sigma^2 (v_\alpha)\sqrt{2n} \right\} \to (1 - \alpha),$$

$$P\left\{ ||\mathbf{\mu} - \hat{\mathbf{\mu}}||^2 \leq \text{SURE} + \sigma^2 (v_{-\alpha})\sqrt{2n} \right\} \to (1 - \alpha)$$

where $v_\alpha, v_{-\alpha}$ are defined in Theorem 3.4.

Similar to Theorem 3.4, Corollary 3.5 provides confidence regions for the entire vector $\mathbf{\mu}$ with exact asymptotic quantiles. Under the condition (3.21), $\text{SURE}$ incurs an error characterized by the quantiles of the random variable $||\varepsilon||^2 - \sigma^2 n$.

We will verify in Theorems 3.11 and 3.13 that the condition (3.21) holds for the Lasso under commonly imposed regularity conditions in sparse regression theory.

Alternatively to Corollary 3.5, the following result replaces the condition on $\gamma_n$ in (3.21) by a data-driven surrogate $\gamma_n$ and provides non-asymptotic interval estimates for both $E[||\hat{\mathbf{\mu}} - \mathbf{\mu}||^2]$ and $||\hat{\mathbf{\mu}} - \mathbf{\mu}||^2$. 
Theorem 3.6. Suppose \( \hat{\mu} \) is 1-Lipschitz and \( \nabla \hat{\mu}(y) \) is almost surely symmetric positive semi-definite. Let \( \text{SURE} \) be as in (3.7). Then,

\[
\text{Var}(\text{SURE} - \text{SURE}[\hat{\mu}^2] + (n\sigma^2 - \|\varepsilon\|^2) \leq 4\text{E}[\sigma^2 \text{SURE} + \sigma^2 d^f],
\]

where \( d^f = \text{div} \hat{\mu} \). Moreover, there exist non-negative random variables \( X_n \) and \( Y_n \) with \( \text{E}[X_n^2] = \text{E}[Y_n^2] = 1 \) such that

\[
\begin{align*}
sure - \text{SURE}[\hat{\mu}^2] + (n\sigma^2 - \|\varepsilon\|^2) \leq 4\text{E}[\sigma^2 \text{SURE} + \sigma^2 d^f],
\end{align*}
\]

where \( \hat{\gamma}_n = 4\text{SURE}/(n\sigma^2) + \text{trace}[\nabla \hat{\mu}] / n \). Consequently for positive \( \alpha, \beta_1 \) and \( \beta_2 \) with \( \alpha + \beta_1 + \beta_2 = \delta < 1 \) and \( \kappa_{n, \beta_2} = 2(6/(\beta_2 n))^{1/4} + 4/(\beta_2 n)^{1/2}, \)

\[p\left\{ \text{SURE} - \text{SURE}[\hat{\mu}^2] \leq v_\alpha + \hat{\gamma}_n^{1/2} + \kappa_{n, \beta_2} \right\} \geq 1 - \delta.
\]

Moreover, (3.23) and (3.24) still hold with \( \text{SURE}[\hat{\mu}^2] \) replaced by \( \|\mu - \hat{\mu}\|^2 \).

As discussed in Remark 3.3, the conclusions of Theorem 3.6 are applicable to all convex penalized estimators in linear regression. Note that \( \hat{\gamma}_n \) is a biased estimate of the left hand side of (3.21) in general due to \( \text{trace}[\{\nabla \hat{\mu}\}^2] \leq \text{trace} \nabla \hat{\mu} \). The estimate \( \hat{\gamma}_n \) involves \( d^f = \text{trace}[\nabla \hat{\mu}] \) instead of \( \text{trace}[\{\nabla \hat{\mu}\}^2] \) because controlling the variance of \( d^f \) easily follows from Section 2.3, while we are not aware of available tools to bound the variance of \( \text{trace}[\{\nabla \hat{\mu}\}^2] \) except in specific cases where \( \nabla \hat{\mu} \) is a projection. The proofs of Theorem 3.4, Corollary 3.5 and Theorem 3.6 are given in Appendix C.

### 3.3. Oracle inequalities for SURE-tuned estimates

Beyond pairwise comparisons, the following result provides guarantees on the SURE-tuned estimate \( \hat{\mu} \), which is obtained by selecting the estimator among \( \hat{\mu}^{(1)}, ..., \hat{\mu}^{(m)} \) with the smallest \( \text{SURE} \), i.e.,

\[
\hat{\mu} = \hat{\mu}^{(k)} \text{ with } k = \arg\min_{j \in [m]} \text{SURE}(j),
\]

where \( \text{SURE}(j) = \|\hat{\mu}^{(j)} - y\|^2 + 2\sigma^2 \text{ trace } \nabla \hat{\mu}^{(j)} - n\sigma^2 \) for \( \varepsilon \sim N(0, \sigma^2 I_n) \).

**Theorem 3.7.** Consider the sequence model \( y = \mu + \varepsilon \) with \( \varepsilon \sim N(0, \sigma^2 I_n) \). Let \( \hat{\mu}^{(1)}(y), ..., \hat{\mu}^{(m)}(y) \) be all L-Lipschitz functions of \( y, \hat{\mu} \) the SURE tuned estimator in (3.25), \( j_0 = \arg\min_{j = 1, ..., m} \text{E}[\|\hat{\mu}^{(j)} - \mu\|^2, s^* = \max_{k \in [m]} \text{E}[\text{trace} ((\nabla \hat{\mu}^{(k)} - \nabla \hat{\mu}^{(j_0)})^2)]. \)

(i) For any \( \alpha \in (0, 1) \), with probability at least \( 1 - \alpha \),

\[
\text{SURE}(j_0) - \text{SURE}(j) \leq \sigma \max \{ 8s^*/m^2, 8s^*(\sqrt{2L} + 1)/m^2 \}.
\]

(ii) For any \( \alpha \in (0, 1) \), with probability at least \( 1 - \alpha \),

\[16\text{SURE}(j_0) - \text{SURE}(j) \leq \sigma \max \{ 8s^*/m^2, 8s^*(\sqrt{2L} + 1)/m^2 \}.
\]
(ii) For any δ ∈ (0, 1), with probability at least 1 − δ,
\begin{equation}
\|\hat{\mu}^{(j)} - \mu\| - \min_{j \in [m]} \|\hat{\mu}^{(j)} - \mu\| \leq 2L\sigma \sqrt{2 \log(m/\delta)}
\end{equation}
so that the sum of (3.26) and (3.27) provide high probability bounds on
\|\hat{\mu} - \mu\| - \min_{j \in [m]} \|\hat{\mu}^{(j)} - \mu\|.
(iii) For some absolute constant C > 0, in expectation
\begin{equation}
E\left[\|\hat{\mu} - \mu\| - \min_{j \in [m]} \|\hat{\mu}^{(j)} - \mu\|\right]^{1/2} \leq C\sigma [\left(s^*m\right)^{1/4} + (1 + L)m^{1/2}].
\end{equation}
(iv) If \( \max_{j \in [m]} E[\|\hat{\mu}^{(j)} - \mu\|^2]/n \leq \sigma^2 \) then the squared risk enjoys
\begin{equation}
E[\|\hat{\mu} - \mu\|^2] - \min_{j \in [m]} E[\|\hat{\mu}^{(j)} - \mu\|^2] \leq \sigma^2(32nm)^{1/2}.
\end{equation}

The proof is given in Appendix D. The assumption that the estimators \( \hat{\mu}^{(j)} \)
are \( L \)-Lipschitz functions of \( y \) is mild, cf. Remark 3.3. Under this assumption,
\( s^* \leq 4L^2n \) and (3.28) implies
\begin{equation}
\frac{\|\hat{\mu} - \mu\|}{n^{1/2}} - \min_{j \in [m]} \frac{\|\hat{\mu}^{(j)} - \mu\|}{n^{1/2}} \leq C\sigma(1 + L) \max \left\{ \left( \frac{m}{\alpha n} \right)^{1/4}, \left( \frac{m}{n\alpha} \right)^{1/2} \right\}
\end{equation}
with probability \( 1 - \alpha \) for some absolute \( C > 0 \), where we used the \( n^{-1/2} \) scaling
to feature the normalized prediction risk \( \|\hat{\mu} - \mu\|^2/n \). Theorem 3.7 (i) can also
be understood in terms of sample size requirement: If \( \epsilon > 0 \) is a fixed precision
target and \( \alpha \in (0, 1) \) then \( n \geq \epsilon^{-2} \max\{m/\alpha, (s^*m/\alpha)^{1/2}\} \) samples are sufficient
to ensure
\[ P\left\{ n^{-1/2}\|\hat{\mu} - \mu\| - \min_{j \in [m]} n^{-1/2}\|\hat{\mu}^{(j)} - \mu\| \leq \sigma\epsilon \right\} \geq 1 - \alpha. \]

We are not aware of a previous result of this form that applies with the above
level of generality, i.e., with no restriction on the nature of the estimators
\( \{\hat{\mu}^{(1)}, ..., \hat{\mu}^{(m)}\} \) beyond the Lipschitz requirement. As shown in the next
proposition, the dependence in \( s^* \) in the term \( (s^*m/\alpha)^{1/4} \) of (3.26) and the dependance in \( n \) in the term \( (m/(n\alpha))^{1/4} \) of (3.30) are unimprovable without
additional assumptions.

**Proposition 3.8.** There exist absolute constants \( C_1, C_2, C_3 > 0 \) such that for
any \( n \geq C_1 \), there exist \( \mu \in \mathbb{R}^n \) and two estimators \( \hat{\mu}^{(1)}(y), \hat{\mu}^{(2)}(y) \) that are
\( L \)-Lipschitz functions of \( y \) such that \( s^* = n \) and \( \hat{\mu} \) in (3.25) satisfies
\[ P\{\|\hat{\mu} - \mu\| - \min_{j=1,2} \|\hat{\mu}^{(j)} - \mu\| \geq C_2\sigma n^{1/4}\} \geq C_3. \]

Oracle inequalities stronger than (3.30) are available if the estimators
\( \{\hat{\mu}^{(j)}, j = 1, ..., m\} \) are affine in \( y \), i.e., of the form \( \hat{\mu}^{(j)} = A_j y + b_j \) for
deterministic \( A_j \in \mathbb{R}^{n \times n} \) and \( b_j \in \mathbb{R}^n \). In this case, \( \text{sOR}^{(j)} = \|\hat{\mu}^{(j)} - y\|^2 + \)
2σ² \text{trace } A_j - nσ² reduces to Mallows C_p [Mal73] and if \( \tilde{\mu} \) is the estimate among \( \{ \hat{\mu}^{(j)}, j \in [m] \} \) with the smallest SURE, then
\[
\mathbb{E}[\| \tilde{\mu} - \mu \| - \min_{j \in [m]} \| \hat{\mu}^{(j)} - \mu \|] \leq C(1 + L)σ(log m)^{1/2}
\]
for some absolute constant \( C > 0 \), provided that the operator norm of \( A_j \) is less than \( L \) for all \( j \in [m] \), cf. [Bel18, Proposition 3.1] or [AB09, TR18] for related results. If \( b_j = 0 \) for all \( j \) and the matrices \( A_j \) are symmetric and totally ordered in the sense of positive semi-definite matrices, the right hand side in (3.31) can even be reduced to \( O(σ) \) [Kne94, BY19]. Equation (3.31) provides an oracle inequality with respect to the risk \( \| \tilde{\mu} - \mu \| \); oracle inequalities of form (3.29) with respect to the squared risk are studied in [LB06, DS12] using exponential weights procedures, and in [DRZ12, DRLT14] [Bel18, Theorem 2.1] using a convex relaxation of SURE named Q-aggregation and introduced in [Rig12]. For linear estimators, these works exhibit an error term involving \( log m \) thanks to the availability of the Hanson-Wright inequality, which provides exponential concentration bounds for random variables of the form \( \varepsilon^\top (A_j - A_k) \varepsilon \).

As the optimal remainder term for an oracle inequality of the form (3.29) satisfied by any estimator of the form \( \hat{\mu}^{(j)}, j \in [m] \) is of order \( σ^2(n \log m)^{1/2} \) for deterministic vectors \( \hat{\mu}^{(j)} = b_j \) [RT12, Theorem 2.1], the dependence in \( n \) of (3.29) is optimal when \( m \) is smaller than an absolute constant.

Compared to these existing results, the novelty of Theorem 3.7 lies in its scope: Theorem 3.7 and (3.30) are applicable to any collection of \( L \)-Lipschitz non-linear estimators \( \{ \hat{\mu}^{(j)}, j \in [m] \} \). The \( L \)-Lipschitz assumption is mild—cf. Remark 3.3—and Theorem 3.7 is thus applicable far beyond the case of linear estimators studied in the aforementioned literature.

A drawback of Theorem 3.7 compared to (3.31) is the sub-optimality of the dependence in \( m \). The difficulty to obtain a rate logarithmic in \( m \) is due to the unavailability of exponential concentration inequalities for random variables of the form \( \varepsilon^\top (\hat{\mu}^{(j)} - \hat{\mu}^{(k)}) \) for non-linear \( \hat{\mu}^{(j)}, \hat{\mu}^{(k)} \).

Finally, we note that an oracle inequality for the squared risk can be obtained using the Q-aggregation procedure from [Rig12, DRZ12, DRLT14] and its analysis in [Bel18]. Indeed, let \( \hat{\mu}_Q = \sum_{j=1}^{m} \theta_j \hat{\mu}^{(j)} \) where
\[
\hat{\theta} = \arg \min_{\theta \succeq 0, 1^\top \theta = 1} \left[ \| \hat{\mu}_\theta - y \|^2 + 2σ^2 \sum_{j=1}^{m} \theta_j \div \hat{\mu}^{(j)} + \frac{1}{2} \sum_{j=1}^{m} \theta_j \| \hat{\mu}^{(j)} - \hat{\mu}_\theta \|_2^2 \right]
\]
and \( \hat{\mu}_\theta = \sum_{j=1}^{m} \theta_j \hat{\mu}^{(j)} \) for every \( \theta \) in the simplex \( \{ \theta \in \mathbb{R}^m : \theta \geq 0, 1^\top \theta = 1 \} \) in \( \mathbb{R}^m \). Then \( \hat{\mu}_Q \) satisfies under the assumptions of Theorem 3.7
\[
\mathbb{E}[\| \hat{\mu}_Q - \mu \|_2^2] - \min_{k \in [m]} \mathbb{E}[\| \hat{\mu}^{(k)} - \mu \|_2^2] \leq 2σ^2 \left( \sqrt{s^*m + (1 + L)^2m} \right) + σ^2 L^2.
\]
We refer to [DRZ12, DRLT14, Bel18] for details on the construction of \( \hat{\mu}_Q \). The proof of (3.32) is given at the end of Appendix D.
3.4. The variance of the model size of the Lasso

Consider a linear regression model

\[(3.33) \quad y = X\beta + \epsilon,\]

where \(\beta\) is the true coefficient vector, \(\epsilon \sim \mathcal{N}(0, \sigma^2 I_n)\) is the noise and \(X\) is a deterministic design matrix. Consider the Lasso which solves the optimization problem

\[(3.34) \quad \hat{\beta}^{(\lambda)} = \arg\max_{b \in \mathbb{R}^p} \{\|Xb - y\|^2/(2n) + \lambda\|b\|_1\}.\]

Let \(\hat{S} = \{j \in [p] : (\hat{\beta}^{(\lambda)}_{\text{lasso}})_{j} \neq 0\}\) be the support of the Lasso. We are interested in the size of \(\hat{S}\) denoted by \(|\hat{S}|\). Even though the Lasso and sparse linear regression have been studied extensively in the last two decades, little is known about the stochastic behavior of the discrete random variable \(|\hat{S}|\). Under the sparse Riesz or similar conditions, \(|\hat{S}| \lesssim \|\beta\|_0\) with high probability \([ZH08, Zha10, ZZ12]\) but such results only imply a bound of the form \(\text{Var}[|\hat{S}|] \lesssim \|\beta\|^2_0\) on the variance; we will see below that the variance of \(|\hat{S}|\) is typically much smaller. There are trivial situations where the behavior of \(|\hat{S}|\) is well understood: if \(\lambda\) is very large for instance, then \(|\hat{S}| = 0\) with high probability. Or, under strong conditions on \(X\) and \(\beta\) that grants support recovery (cf. for instance, the conditions given in \([MB06, ZY06, Tro06, Wai09]\)), \(\hat{S} = \text{supp}(\beta)\) holds with probability at least \(1 - 1/p^2\) and in this case \(\text{Var}[|\hat{S}|] \leq \mathbb{E}[(|\hat{S}| - s_0)^2] \leq 1\).

Outside of these situations, studying \(|\hat{S}|\) appears delicate; for instance, our previous attempts at studying the variance of \(|\hat{S}|\) went as follows. Let \((e_1, ..., e_p)\) be the canonical basis in \(\mathbb{R}^p\) and let \(x_j = Xe_j\) for all \(j = 1, ..., p\). The KKT conditions of the Lasso are given by

\[
x_j^\top(y - X\hat{\beta}^{(\lambda)}_{\text{lasso}})/(n\lambda) \begin{cases} = \text{sgn}((\hat{\beta}^{(\lambda)}_{\text{lasso}})_j) & \text{if } (\hat{\beta}^{(\lambda)}_{\text{lasso}})_j \neq 0, \\ \in [-1, 1] & \text{if } (\hat{\beta}^{(\lambda)}_{\text{lasso}})_j = 0. \end{cases}
\]

At a given point \(y\), to understand the stability of \(\hat{S}\), a natural avenue is to identify how close the quantities \(x_j^\top(y - X\hat{\beta}^{(\lambda)}_{\text{lasso}})/(n\lambda)\) are from \(\pm 1\) for the indices \(j \notin \hat{S}\). If many indices \(j \notin \hat{S}\) are such that \(x_j^\top(y - X\hat{\beta}^{(\lambda)}_{\text{lasso}})/(n\lambda)\) is extremely close to \(\pm 1\), then a tiny variation in \(y\) may push some of the quantities \(x_j^\top(y - X\hat{\beta}^{(\lambda)}_{\text{lasso}})/(n\lambda)\) towards \(\pm 1\) resulting in many new variables entering the support for this tiny variation in \(y\). The current model size \(|\hat{S}|\) is non-informative about how many indices \(j \notin \hat{S}\) are such that \(x_j^\top(y - X\hat{\beta}^{(\lambda)}_{\text{lasso}})/(n\lambda)\) is extremely close to \(\pm 1\) and the random variable \(|\hat{S}|\) appears prone to instability.

With the Second Order Stein formula \((2.3)\) and the tools developed in the previous section, the variance of \(|\hat{S}|\) can be bounded as follows. First, we need to describe a condition on the deterministic matrix \(X\) which ensures that the
KKT conditions of the Lasso hold strictly with probability 1. We say that the KKT conditions hold strictly if
\begin{equation}
\forall j \notin \hat{S}, \quad -1 < \frac{1}{\lambda n} x_j^T (y - X \hat{\beta}_{\text{lasso}}^{(\lambda)}) < 1.
\end{equation}

**Assumption 3.1.** For all \( \delta_1, ..., \delta_p \in \{-1, 1\} \) and \( 1 \leq j_0 < j_1 < \cdots < j_n \leq p, \)
\[
\text{rank}( \begin{pmatrix} x_{j_0} & x_{j_1} & \cdots & x_{j_n} \\ \delta_{j_0} & \delta_{j_1} & \cdots & \delta_{j_n} \end{pmatrix})_{(n+1) \times (n+1)} = n + 1.
\]

**Proposition 3.9.** If \( X \) satisfies the above assumption then the set \( B = \{ j \in [p] : |x_j^T (y - X \hat{\beta}_{\text{lasso}}^{(\lambda)})| = \lambda n \} \) is such that \( X_B \) has rank \( |B| \) and the solution \( \hat{\beta}_{\text{lasso}}^{(\lambda)} \) to the optimization problem (3.34) is unique. Furthermore, if \( P[v^T \epsilon = c] = 0 \) for all vectors \( v \neq 0 \) and real \( c \), then the KKT conditions of the Lasso \( \hat{\beta}_{\text{lasso}}^{(\lambda)} \) hold strictly with probability 1, i.e., (3.35) holds with probability 1.

Expositions of the results in the first part of the above proposition exist in the literature, see for instance [Zha10, Section 3] or [TT12, Tib13]. Compared with previous versions of the condition on the design, Assumption 3.1, which clearly holds with probability 1 when \( X \) is the realization of a continuous distribution over \( \mathbb{R}^{n \times p} \), gives a natural interpretation in terms of the rank of specific matrices. The fact that the KKT conditions of the Lasso hold strictly with probability 1 is known although it is difficult to pinpoint an existing result in the form of Proposition 3.9 in the literature. We provide a short proof in Appendix E for completeness.

Next define the function \( f : \mathbb{R}^n \to \mathbb{R}^n \) by
\begin{equation}
f : \epsilon \to X (\hat{\beta}_{\text{lasso}}^{(\lambda)} - \beta).
\end{equation}

Then the function \( f \) is 1-Lipschitz and this property holds true for all convex penalized Least-Squares estimators [BT17, Proposition 3]. Consequently, almost everywhere the partial derivatives of \( f \) exist and \( \nabla f(\epsilon) \) has operator norm at most one. It is enough to compute the gradient of \( f \) Lebesgue almost everywhere and by the above proposition, the KKT conditions holds strictly for almost every point \( \epsilon_0 \in \mathbb{R}^n \).

If the KKT conditions of the Lasso hold strictly for \( \epsilon_0 \), then by Lipschitz continuity of \( \epsilon \to X \hat{\beta}_{\text{lasso}}^{(\lambda)} \), the KKT conditions also hold strictly in small enough nontrivial neighbourhood of \( \epsilon_0 \). In this small neighborhood, the sign and support of \( \hat{\beta}_{\text{lasso}}^{(\lambda)} \) are unchanged and we have for \( \| \epsilon \| \) small enough
\[
X \hat{\beta}_{\text{lasso}}^{(\lambda)} (\epsilon_0 + \epsilon) = X_{\hat{S}} (X_{\hat{S}}^T X_{\hat{S}})^{-1} (X_{\hat{S}}^T (\epsilon_0 + \epsilon) + X \beta) - \lambda \text{sign}(\hat{\beta}_{\text{lasso}}^{(\lambda)} (\epsilon_0)),
\]
where \( \hat{S} \) denotes the locally constant support equal to the support of \( \hat{\beta}_{\text{lasso}}^{(\lambda)} (\epsilon_0) \). In this neighbourhood the map \( \epsilon \to X \hat{\beta}_{\text{lasso}}^{(\lambda)} (\epsilon_0 + \epsilon) \) as well as the map \( \epsilon \to X (\hat{\beta}_{\text{lasso}}^{(\lambda)} (\epsilon_0 + \epsilon) - \beta) \) are locally affine with linear part equal to the orthogonal projection
\begin{equation}
P_{\hat{S}} = X_{\hat{S}} (X_{\hat{S}}^T X_{\hat{S}})^{-1} X_{\hat{S}}^T.
\end{equation}

We conclude this calculation with the following lemma.
Theorem 3.11. Consider the linear model (3.33) and Appendix F. Using Theorem 2.2 we obtain the following result whose proof is given in 3.4.1. Variance formula and relative stability

**Proposition 3.10.** Let \( \hat{\beta}_{lasso}^{(\lambda)} \) be the Lasso estimator (3.34) with data \((X, y)\) satisfying \( y = X\beta + \varepsilon \). Define \( f(\varepsilon) = X(\hat{\beta}_{lasso}^{(\lambda)} - \beta) \) as in (3.36). Suppose Assumption 3.1 holds and \( P\{v^\top \varepsilon = c\} = 0 \) for all deterministic \( v \in \mathbb{R}^n \) and real \( c \). Then almost surely

\[
\nabla \hat{\beta}_{lasso}^{(\lambda)} = \begin{pmatrix} (X_S^\top X_S)^{-1}X_S^\top \varepsilon \\ 0_{p \times n} \end{pmatrix}_{p \times n}
\]

as well as

\[
\nabla f(\varepsilon) = P_S \quad \text{and} \quad \text{div } f(\varepsilon) = \|P_S\varepsilon\|^2_F = \text{trace } P_S = |\hat{S}|,
\]

where \( \hat{S} = \text{supp}(\hat{\beta}_{lasso}^{(\lambda)}) \) and \( P_S \) is as in (3.37).

3.4.1. Variance formula and relative stability

Using Theorem 2.2 we obtain the following result whose proof is given in Appendix F.

**Theorem 3.11.** Consider the linear model (3.33) and \( \hat{\beta}_{lasso}^{(\lambda)} \), in (3.34), with deterministic design \( X \) satisfying Assumption 3.1, true target vector \( \beta \) and noise \( \varepsilon \sim N(0, \sigma^2 I_n) \). Then the variance of the size of the selected support satisfies

\[
\text{Var}[|\hat{S}|] = \mathbb{E}[|\hat{S}|] + \mathbb{E}[\|P_S\varepsilon\|^2/\sigma^2] + \text{Var}(g(\varepsilon)) - \sigma^2 \mathbb{E}[\|\nabla g(\varepsilon)\|^2]
\]

\[
\leq \mathbb{E}[|\hat{S}|] + \mathbb{E}[\|P_S\varepsilon\|^2/\sigma^2],
\]

(3.38)

where \( g(\varepsilon) = \varepsilon^\top X(\hat{\beta}_{lasso}^{(\lambda)} - \beta)/\sigma^2 \). Consequently, \( \text{Var}[|\hat{S}|] \leq 2n \) as well as

\[
\text{Var}[|\hat{S}|] \leq \mathbb{E}[|\hat{S}|] + 4 \mathbb{E}[|\hat{S}|] \log \left( \frac{e^p}{1\sqrt{\mathbb{E}[\|\hat{S}\|]}} \right)
\]

\[
\leq \mathbb{E}[|\hat{S}|] + 4 \mathbb{E}[|\hat{S}|] \log \left( \frac{e^p}{1\sqrt{\mathbb{E}[\|\hat{S}\|]}} \right).
\]

A significant feature of the above theorem, and Theorem 2.2 as well, is the requirement of no condition on the true \( \beta \), the penalty level \( \lambda \) or the design matrix \( X \) beyond Assumption 3.1. In particular, the restricted eigenvalue condition is not required.

Using \( a/b + b/(a \lor 1) - 2 \leq (a - b)^2/(b(a \lor 1)) \), an implication of Theorem 3.11 is the confidence interval

\[
\mathbb{P} \left( \frac{|\hat{S}|}{\mathbb{E}[|\hat{S}|]} + \frac{\mathbb{E}[|\hat{S}|]}{|\hat{S}| \lor 1} - 2 \leq C_\alpha \left( \frac{3}{|\hat{S}| \lor 1} + \frac{4\log(ep)}{|\hat{S}| \lor 1} \right) \right) \geq 1 - \alpha
\]

(3.40)

for \( \mathbb{E}[|\hat{S}|] \) with conservative \( C_\alpha = 1/\alpha \), although \( \mathbb{E}[|\hat{S}|] \) is not a conventional parameter due to its dependence on the specific choice of \( \hat{\beta} \).

A sequence of non-negative random variables \( (Z_q)_{q \geq 1} \) is said to be relatively stable if \( Z_q/\mathbb{E}[Z_q] \) converges to 1 in probability. A direct consequence of
Theorem 3.11 is that the model size $|\hat{S}|$ is relatively stable provided that $E[|\hat{S}|]$ is not pathologically small. If the setting and assumptions of Theorem 3.11 are fulfilled then

$$E\left[\left(\frac{|\hat{S}|}{E|\hat{S}|} - 1\right)^2\right] \leq \frac{3}{E|\hat{S}|} + \frac{4\log(ep/E|\hat{S}|)}{E|\hat{S}|} \leq \frac{3 + 4\log(ep)}{E|\hat{S}|}.$$

Consequently, if one considers a sequence of regression problems such that $E[|\hat{S}|]/\log(ep) \to +\infty$, then $|\hat{S}|/E|\hat{S}|$ converges to 1 in $L_2$ and in probability. It is known that $P\{|\hat{S}| \geq k\} \approx 1$ when $X$ has iid $N(0, \Sigma)$ rows with $(\Sigma)_{jj} = 1$, $\beta = 0$ and $\lambda = \lambda(k) = (\sigma/n^{1/2})\{L(k/p) - 1\}$ under a mild side condition on $\Sigma$, where $L(t)$ is defined by $P\{N(0, 1) > L(t)\} = t$ [SZ13][Proposition 14(ii)]. As $|\hat{S}|$ is expected to be larger when $\beta \neq 0$, it would be reasonable to expect $E[|\hat{S}|] \gg \log p$ when $\lambda = \lambda(k_n)$ with $k_n \gg \log p$.

An informative benchmark to study the tightness of inequality (3.39) for the support of the Lasso is the case $X = \sqrt{n}I_p$ which reduces to the Gaussian sequence model. Then $\beta_{lasso}^{(\lambda)}$ is the soft-thresholding operator and $|\hat{S}|$ is the sum of $p$ iid Bernoulli random variables with parameters $q_1, \ldots, q_p \in (0, 1)$ and $Var[|\hat{S}|] = \sum_{j=1}^{p} q_j (1 - q_j)$. Under mild assumption on the probabilities $q_j$ (e.g., $q_j \leq 1/2$ for all $j$), the variance $Var[|\hat{S}|]$ is of the same order as $E[|\hat{S}|]$. Hence the bound (3.39) is sharp up to a logarithmic factor.

### 3.4.2. Linearity of the variance in the true model size

From (3.39), we can also obtain more explicit bounds on the variance of $|\hat{S}|$ by bounding from above $E[|\hat{S}|]$. We provide below upper bounds on $E[|\hat{S}|]$ under two assumptions on $X$: the Sparse Riesz Condition (SRC) [ZH08, Zha10] and the Restricted Eigenvalue (RE) condition [BRT09]. Under both conditions, if the tuning parameter of the Lasso is large enough then the squared risk $\|X(\beta_{lasso} - \beta)\|^2/n$ is bounded from above by $C(X)s_0\lambda^2$ with high probability [ZH08, BRT09, Zha10] and in expectation [YZ10, BLT18, BT17], where $C(X)$ is a multiplicative constant that depends on $X$. We refer the reader to the books [BVDG11, GHV12, HTW15] and the references therein for surveys of existing results. Throughout the rest of this section, denote by $s_0 = ||\beta||_0$ the number of nonzero coefficients, or sparsity, of the unknown coefficient vector $\beta$.

The Sparse Riesz Condition (SRC) [ZH08, Zha10] on the design $X$ holds if for certain $\eta \in (0, 1)$ and nonnegative reals $\{\epsilon_1, \epsilon_2\}$ and integers $\{m, k\}$,

$$|S| + \epsilon_2 k \leq \min_{B \subset [p]: |B| \leq m} \frac{2(1 - \eta)^2m - \epsilon_1 k}{\phi_{\text{cond}}(X_B^T X_B) - 1},$$

where $S$ denotes the support of $\beta$ and $\phi_{\text{cond}}(\cdot)$ denotes the condition number. Let $\phi(d) \geq \max\{\phi_{\text{cond}}(X_B^T X_B): |B| = d\}$ be an upper bound for the $d$-sparse condition number of the Gram matrix $X^T X/n$. Given $d$ and $\{\eta, \epsilon_1, \epsilon_2\}$, the SRC can be viewed as a sparsity condition on $\beta$ as it holds with $k = ||\beta||_0$. 


when $\|\beta\|_0 \leq 2d(1 - \eta^2)/(1 + \epsilon_2)(\phi(d) - 1) + 2(1 - \eta^2) + \epsilon_1$. In particular, the SRp holds under the RIP condition $\delta_{2s_0} < 1/2$ or $\delta_{3s_0} < 2/3$ for sufficiently small $\{\eta, \epsilon_1, \epsilon_2\}$ where $\delta_1$ is the maximum spectrum norm of $X_B^T X_B/n - I_B$ over $|B| \leq k$. When $X$ has iid $N(0, \Sigma)$ rows, we may take $d = a_1 n / \log p$ such that $\phi(d) = (1 + a_2)\phi_{\text{cond}}(\Sigma)$ is a valid upper bound for the $d$-sparse condition number of $X^T X/n$ with probability $1 - e^{-a_2 n}$ for some small positive constants $a_1$ and $a_2$ [ZH08].

Note that the original SRC in [ZH08] is stated in terms of ratio of maximal and minimal sparse eigenvalues instead of sparse condition number as in (3.41). A common feature on the works on the SRC [ZH08, Zha10] is that $|S| \lesssim s_0$ with large probability (up to constants depending on the SRp constants and the tuning parameter). We obtain $\mathbb{E}[|\hat{S}|] \lesssim s_0$ as a consequence, provided that $\mathbb{P}(|\hat{S}| \lesssim s_0)$ is large enough.

**Proposition 3.12.** Let $\varepsilon \sim N(0, \sigma^2 I_n)$ and $s_0 = \|\beta\|_0$ in the linear model (3.33). Let the tuning parameter of the Lasso (3.34) satisfy

$$
(3.42) \quad \lambda \geq (\sigma/\eta) \sqrt{(1 + \tau)(2/n) \log(p/k)}
$$

with $\eta \in (0, 1)$. Assume that $X$ is deterministic with $\max_{j \in [p]} |X e_j|^2 / n \leq 1$ and that (3.41) holds with $\epsilon_1 = 8(1 - \eta)/(\sqrt{2} t_0)$, $\epsilon_2 = 4/(\{t_0^2(2p^2 + 4)^{1/2}\}^{1/2})$ and some nonnegative integers $\{m, k\}$, such that $t_0 = \eta^{-1} \sqrt{2 \log(p/k)}$, then $\mathbb{P}(S \setminus S) < m$ and $0 < \eta^2 \leq 1/2$. The proof is given in Appendix H. In particular if $\tau \geq 1$ and $s_0 = 2m$ and $k \lesssim 1$, then the SRC grants $\mathbb{E}[|\hat{S}|] \lesssim s_0$. The expectation $\mathbb{E}[|\hat{S}|]$ can also be bounded from above if both Assumption 3.1 and the Restricted Eigenvalue (RE) condition [BRT09] hold.

**Theorem 3.13.** Consider the linear model (3.33) with $\varepsilon \sim N(0, \sigma^2 I_n)$ and $s_0 = \|\beta\|_0$. Let $\tau, \gamma > 0$, $\omega = \sigma(1 + \tau)/\sqrt{n}$ and $\hat{\beta}^{(s_0)}$ be as in (3.34) with

$$
(3.43) \quad \lambda = \sigma(1 + \tau)(1 + \gamma) \sqrt{(2/n) \log(p/(s_0 \lor 1))}.
$$

Assume that the columns of $X$ are normalized such that $\max_{j \in [p]} |X e_j|^2 \leq n$. Let $\hat{S}$ be the support of $\hat{\beta}^{(s_0)}$. Then the Lasso satisfies

$$
\mathbb{E}\left[ 2\varepsilon^T X (\hat{\beta}^{(s_0)} - \beta) + \|X (\hat{\beta}^{(s_0)} - \beta)\|^2 / n \right] \leq \frac{s_0(\lambda^2 + \omega^2) + (s_0 \lor 1) \omega^2}{\text{RE}^2(S, c_0)} + \frac{\omega^2}{2},
$$

where $\text{RE}(S, c_0) = \inf_{u \in \mathbb{R}^n : \|u\|_1 \leq c_0 \sqrt{n}} \|n^{-1/2} X u\| / \|X u\|$ and $S$ is the support of $\beta$, provided that $c_0 \geq \gamma^{-1} \sqrt{2(1 + 2\omega^2/\lambda^2)}$, e.g. $c_0 = 2/\gamma$. If in addition Assumption 3.1 holds, then

$$
(3.44) \quad \mathbb{E}\left[ |\hat{S}| + \|X (\hat{\beta}^{(s_0)} - \beta)\|^2 / (2\sigma^2 \tau) \right] \leq \left( \sqrt{\tau} + 1/\sqrt{\tau} \right)^2 \left[ (1 + \gamma)^2 \left\{ s_0 \log(p/(s_0 \lor 1)) + (s_0 \lor 1) \right\} + \frac{1}{4} \right].
$$
The proof of Theorem 3.13 is given in Appendix I. The Gaussian concentration theorem is used in [BT17, BLT18] to obtain bounds on $\mathbb{E}[\|X(\hat{\beta}^{(\lambda)}_{\text{asso}} - \beta)\|^2]$ as well as higher order moments of the squared risk; similar arguments are used to derive Theorem 3.13. If $X$ satisfies Assumption 3.1 then $\mathbb{E}[e^\top X(\hat{\beta}^{(\lambda)}_{\text{asso}} - \beta)] = \mathbb{E}[\hat{S}]$, so that the argument leads to (3.44). Informally, this implies $\mathbb{E}[\hat{S}] \lesssim 1 + s_0 \log(ep/(s_0 \vee 1))$ up to a multiplicative constant that depends only on $\gamma, \tau$ and the restricted eigenvalue. To our knowledge, this bound on the size of the model selected by the Lasso under the RE condition is new.

Previous upper bounds of the form $|\hat{S}| \lesssim s_0$ require that both maximal and minimal sparse eigenvalues of $X^\top X/n$ are bounded away from 0 and $\pm \infty$, cf. Proposition 3.12 above or [ZH08], [Zha10, Lemma 1], [BRT09, (7.9)], [BCW14, Theorem 3] among others. The major difference between such conditions and the RE condition is that the RE condition does not require any bounds on the maximal sparse eigenvalues of $X^\top X/n$. Inequality (3.44) reveals that the RE condition is sufficient to control $\mathbb{E}[|\hat{S}|]$ by $s_0$ a logarithmic factor. Under the RE condition, assumptions on the maximal sparse eigenvalues of $X^\top X/n$ are unnecessary to control $\mathbb{E}[|\hat{S}|]$.

The above bounds on $\mathbb{E}[\hat{S}]$ under the SRC or the RE condition yield the following on the variance of $|\hat{S}|$ in virtue of (3.39). If Assumption 3.1 holds, then:

(i) If $\lambda$ is as in (3.43) for some $\gamma, \tau > 0$ and $\max_{j=1,\ldots,p} \|Xe_j\|^2 \leq n$ then

$$\text{Var}[|\hat{S}|] \leq \frac{(s_0 \vee 1)C}{2 \tau \log\left(\frac{ep}{1 \vee s_0}\right)^2},$$

where $C = C(\gamma, \tau) > 0$ only depends on $\gamma, \tau$.

(ii) If $X$ satisfies the SRC (3.41) for some $\eta > 0$ and $0 \leq m, k \leq p$, with $\lambda$ as in (3.42) with $\tau \geq 1$ then for some absolute constant $C' > 0$,

$$\text{Var}[|\hat{S}|] \leq C' \left((s_0 + m) \log\left(\frac{ep}{s_0 \vee s_0 + m}\right)\right).$$

In other words, under the RE condition or the SRC with $n \approx s_0$ the standard deviation of the size of the model $|\hat{S}|$ is smaller than $\sqrt{s_0}$ up to logarithmic factors. The bound is sharper under the SRC by a logarithmic factor.

3.4.3. Variance of degrees-of-freedom of penalized estimators

Some techniques above are not specific to the Lasso. For instance, for any estimator defined as the solution of a convex optimization problem of the form given in Remark 3.3, the map $f : \varepsilon \to X(\hat{\beta} - \beta)$ is 1-Lipschitz and satisfies

$$\mathbb{E}[(\sigma^2 \hat{df} - \varepsilon^\top f(\varepsilon))^2]) \leq \sigma^2 \mathbb{E}[X(\hat{\beta} - \beta)]^2 + \sigma^4 \mathbb{E}[\nabla f(\varepsilon)^2],$$

(3.45)

by Theorem 2.1 where $\hat{df} = \text{div} f(\varepsilon)$. Similarly, by Theorem 2.2 we have

$$\text{Var}[\hat{df}] \leq \frac{\mathbb{E}[\nabla f(\varepsilon)^2]}{\mathbb{E}[\nabla f(\varepsilon)^2]} + \mathbb{E}[\nabla f(\varepsilon)\varepsilon]^2 / \sigma^2 \leq 2n.$$

(3.46)
3.5. SURE for SURE in high-dimensional linear regression

Again we consider linear regression with deterministic design $X \in \mathbb{R}^{n \times p}$. With the notation of Section 3.1, consider the sequence model $y = \mu + \varepsilon$ where $\varepsilon \sim N(0, \sigma^2 I_n)$ and the unknown mean is $\mu = X\beta$, as in the linear model (3.33).

3.5.1. Lasso

Set $\hat{\mu}(y) = X\hat{\beta}^{(\lambda)}_{\text{lasso}}$ with the Lasso estimator (3.34). We have derived in the previous section the gradient of $\varepsilon \rightarrow X\hat{\beta}^{(\lambda)}_{\text{lasso}}$ almost everywhere under Assumption 3.1. It is instructive to use these calculations to make explicit SURE for SURE from Section 3.1 in the Lasso case. Under Assumption 3.1, $\hat{S} = \text{div} \hat{\mu} = \text{trace}(\nabla \hat{\mu})^2$ by Proposition 3.10, so that Stein’s Unbiased Risk Estimate is

$$\text{SURE} = \|y - X\hat{\beta}^{(\lambda)}_{\text{lasso}}\|^2 + \sigma^2(2|\hat{S}| - n)$$

as in (3.7). Moreover, by Theorem 3.1, SURE for SURE in the Lasso case is

$$\hat{R}_{\text{sure}} = 4\sigma^2\|y - X\hat{\beta}^{(\lambda)}_{\text{lasso}}\|^2 + \sigma^4(4|\hat{S}| - 2n)$$

which is an unbiased estimator of $R_{\text{sure}} = E[(\text{SURE} - \|X(\hat{\beta}^{(\lambda)}_{\text{lasso}} - \beta)\|^2)^2]$. The identity $E[\hat{R}_{\text{sure}}] = R_{\text{sure}}$ for the Lasso appeared previously in [DKF+13].

As $\nabla(X\hat{\beta}^{(\lambda)}_{\text{lasso}}) = P_{\beta}$ is a random projection, Theorem 3.2 applies with $\hat{R}'_{\text{sure}} = \hat{R}_{\text{sure}}$, so that SURE for SURE is consistent. We explicitly state the consequences of this result in the following proposition.

**Proposition 3.14.** Consider the sequence model $y = \mu + \varepsilon$ where $\varepsilon \sim N(0, \sigma^2 I_n)$ and let $X \in \mathbb{R}^{n \times p}$ satisfy Assumption 3.1. Let $\beta^{(\lambda)}_{\text{lasso}}$ be the Lasso (3.34). Consider SURE in (3.47) and SURE for SURE in (3.48). Then for any tuning parameter $\lambda \geq 0$, the following holds:

(i) $\text{Var}(\text{SURE}) = E[(\text{SURE} - E[\|y - X\hat{\beta}^{(\lambda)}_{\text{lasso}}\|^2])^2] \leq E[\hat{R}_{\text{sure}}] + \sigma^4 n$.

(ii) $E[\hat{R}_{\text{sure}}] = 2\sigma^2 E[\|y - X\hat{\beta}^{(\lambda)}_{\text{lasso}}\|^2 + \text{SURE}] \geq n\sigma^4$.

(iii) The self-bounding property $\text{Var}[\hat{R}_{\text{sure}}] \leq 16\sigma^4 E[\hat{R}_{\text{sure}}]$ holds.

(iv) Inequality $E[|\hat{R}_{\text{sure}}/E[\hat{R}_{\text{sure}}] - 1|^2] \leq 16/n$ holds so that the ratio $\hat{R}_{\text{sure}}/E[\hat{R}_{\text{sure}}]$ converges to 1 in $L_2$ and in probability as $n, p \to \infty$.

(v) For any $\alpha, \gamma \in (0, 1)$, with probability at least $1 - \alpha - \gamma$, $|\text{SURE} - \|X\hat{\beta}^{(\lambda)}_{\text{lasso}} - \mu\|^2| \leq \gamma^{-1}\hat{R}_{\text{sure}}(1 - 4(n\alpha)^{-1/2})^{-1}$.

The proof is given in Appendix J. In the above, (i) provides in terms of SURE for SURE an upper bound for the mean squared error of SURE when the prediction risk is viewed as the estimation target of SURE, and (iv) is a consistency result for SURE for SURE in the Lasso case. The non-asymptotic
Proposition 3.14 holds with no restriction on \((n, p)\) and the tuning parameter \(\lambda\). The assumption-free nature of Proposition 3.14 is striking: SURE for SURE is consistent even if the Lasso itself is not consistent for prediction in the sense that \(\E[\|X\wh{\beta}^{(\lambda)} - \mu\|^2/(n\sigma^2)]\) is bounded away from 0.

To bound the variance of \(R_{\text{wffe}}\), Proposition 3.14 (iv) leverages the fact that for \(\wh{\mu}(y) = X\wh{\beta}^{(\lambda)}, \nabla\wh{\mu}(y)\) is a random orthogonal projection and \(R_{\text{wffe}} = R'_{\text{wffe}}, \) cf. the discussion following (3.9). While \(\nabla\wh{\mu}(y)\) for \(\wh{\mu}(y) = X\wh{\beta}(y)\) is not a projection for other estimators \(\wh{\beta}\) such as the Elastic-Net studied in Section 3.5.3, the upper bounds in Theorem 3.2 still apply to \(R'_{\text{wffe}}\) for any convex regularized least-squares as explained in Remark 3.3.

A drawback of the confidence region in (v) is the conservative constant factor \(\gamma^{-1}\). This can be fixed under common regularity assumptions made in sparse linear regression as follows with the approach of Section 3.2. Let \(\{\tau, \gamma, \lambda\}\) be as in Theorem 3.13 and define \(C_{\tau, \gamma} = \max(1, 2\tau)((\sqrt{\tau} + 1/\sqrt{\tau})^2\{4(1 + \gamma)^2 + 5\}\). Under the conditions of Theorem 3.13 including Assumption 3.1, (3.44) implies that the right-hand side of (3.18) is bounded by \(\sigma^2 n\epsilon_n^*/\sigma^2\) with \(\epsilon_n^* = C_{\tau, \gamma}(s_0 \vee 1)(\log(p/(s_0 \vee 1)))/\{nR^2(S, 2/\gamma)\}, \) so that
\[
P\left\{\text{SURE} - \|\mu - \wh{\mu}\|^2 \leq 1.96\sigma^2\sqrt{2n}\right\} \approx 95%
\]
by Theorem 3.4 when \(\epsilon_n^* = o(1)\), with \(\epsilon_n = \sqrt{\epsilon_n^*}\), and similarly
\[
P\left\{\|\mu - \wh{\mu}\|^2 \leq \text{SURE} + 1.645\sigma^2\sqrt{2n}\right\} \approx 95%.
\]

3.5.2. Two or more Lasso estimators

For the comparison of two Lasso estimators \(\wh{\beta}^{(\lambda_1)}\) and \(\wh{\beta}^{(\lambda_2)}\) with \(\lambda_1 \neq \lambda_2\),
\[
\text{SURE} \overset{(\text{diff})}{=} \|X\wh{\beta}^{(\lambda_1)} - y\|^2 - \|X\wh{\beta}^{(\lambda_2)} - y\|^2
+ 2\sigma^2\left(|S^{(\lambda_1)}| - |S^{(\lambda_2)}|\right)
\]
(3.49)
provides \(\E[\text{SURE} \overset{(\text{diff})}{=} \E[\|X(\wh{\beta}^{(\lambda_1)} - \beta)\|^2 - \|X(\wh{\beta}^{(\lambda_2)} - \beta)\|^2]\right\}, \) where \(S^{(\lambda_i)} = \text{supp}(\wh{\beta}^{(\lambda_i)}).\) If \(P_A\) is the projection onto the column space of \(X_A\),
\[
\wh{R} \overset{(\text{diff})}{=} 4\sigma^2\|X(\wh{\beta}^{(\lambda_1)} - \wh{\beta}^{(\lambda_2)})\|^2 + 4\sigma^4\text{trace}\left((P_{\hat{S}^{(\lambda_1)}} - P_{\hat{S}^{(\lambda_2)}})^2\right)
\]
(3.50)
provides
\[
\E\wh{R} \overset{(\text{diff})}{=} R \overset{(\text{diff})}{=} \E\left[\left(\|X(\wh{\beta}^{(\lambda_1)} - \beta)\|^2 - \|X(\wh{\beta}^{(\lambda_2)} - \beta)\|^2 - \text{SURE} \overset{(\text{diff})}{=} \right)^2\right].
\]

The results of Section 3.3 are also directly applicable to SURE-tuned Lasso estimators: If \(\lambda\) is the tuning parameter among \(\{\lambda_1, \ldots, \lambda_m\}\) with the smallest SURE, then for some absolute constant \(C > 0\)
\[
\E\left[n^{-1/2}\|X(\wh{\beta}^{(\lambda)} - \beta)\| - \min_{\lambda \in \{\lambda_1, \ldots, \lambda_m\}} n^{-1/2}\|X(\wh{\beta}^{(\lambda)} - \beta)\| \right] \leq C(m/n)^{1/4}.
\]
3.5.3. Elastic Net

Similar computations can be carried out for other estimators such as the Group Lasso or the Elastic Net. For instance, consider the Elastic Net estimator \( \hat{\beta}_{\text{EN}} \) defined as the solution of the optimization problem

\[
\hat{\beta}_{\text{EN}} = \arg \max_{b \in \mathbb{R}^p} \| Xb - y \|^2 / 2n + \lambda \| b \|_1 + \gamma \| b \|^2 / 2,
\]

where \( \lambda, \gamma > 0 \). Set \( \hat{\mu}(y) = X\hat{\beta}_{\text{EN}} \). Then by similar arguments as in the Lasso case, the KKT conditions of the optimization problem (3.51) hold strictly almost everywhere in \( y \). By differentiating the KKT conditions on a neighbourhood where the KKT conditions hold strictly (the details are omitted), the gradient of \( y \to \beta_{\text{EN}} \) is given by

\[
\nabla \hat{\beta}_{\text{EN}} = \left( \left( \gamma I_\hat{S} + X_\hat{S}^T X_\hat{S} \right)^{-1} X_\hat{S}^T \right)_{p \times n},
\]

and the gradient of \( y \to X\hat{\beta}_{\text{EN}} \) is given by

\[
\nabla(X\hat{\beta}_{\text{EN}}) = X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T.
\]

where \( \hat{S} \subset [p] \) is the set of nonzero coefficients of \( \hat{\beta}_{\text{EN}} \). Stein’s Unbiased Risk Estimate is given by

\[
\text{SURE} = \| y - X\hat{\beta}_{\text{EN}} \|^2 + 2\sigma^2 \text{trace} \left[ X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T \right] - \sigma^2 n,
\]

and SURE for SURE in the Elastic Net case is

\[
\hat{R}_{\text{sure}} = 4\sigma^2 \| X\hat{\beta}_{\text{EN}} - y \|^2 + 4\sigma^4 \| X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T \|^2 - 2\sigma^4 n.
\]

By Theorem 3.1, this is an unbiased estimate of \( \mathbb{E}\{ (\text{SURE} - \| X(\beta - \hat{\beta}_{\text{EN}}) \|^2) \} \). SURE for SURE \( \hat{R}_{\text{sure}} \) for the difference between two E-nets or between the Lasso and E-net can be derived similarly as in (3.50). We omit the details.

Remark 3.4. Let \( \hat{df} = \text{trace}[X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T] \). Since \( \hat{df} \) is the divergence of the function \( \varepsilon \to X(\hat{\beta}_{\text{EN}} - \beta) \), Theorem 2.2 implies that

\[
\text{Var}[\hat{df}] \leq \mathbb{E}\{ \| X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T \|_F \}^2 + \mathbb{E}\{ \| X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T \varepsilon \| \}^2 / \sigma^2.
\]

If \( P_\hat{S} \) is the orthogonal projection onto the span of the columns of \( X_\hat{S} \) then the second term satisfies \( \mathbb{E}\{ \| X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T \varepsilon \| \}^2 / \sigma^2 \leq \mathbb{E}\{ \| P_\hat{S} \varepsilon \|^2 \} / \sigma^2 \). Since the right-hand of (3.38) is no greater than that of (3.39) for any random \( \hat{S} \) by the proof of Theorem 3.11, we obtain

\[
\text{Var}[\hat{df}] \leq \mathbb{E}\{ \| X_\hat{S}(\gamma I_\hat{S} + X_\hat{S}^T X_\hat{S})^{-1} X_\hat{S}^T \|_F \}^2 + \mathbb{E}[2|\hat{S}| + 4|\hat{S}| \log(ep/(1 \lor |\hat{S}|))] + 3\mathbb{E}[|\hat{S}|] + 4\mathbb{E}[|\hat{S}|] \log(ep/(1 \lor |\hat{S}|))].
\]
3.6. De-biasing nonlinear estimators in linear regression

Consider a linear regression model

\[ y = X\beta + \epsilon \]  

with an unknown target vector \( \beta \in \mathbb{R}^p \), a Gaussian noise vector \( \epsilon \sim N(0, \sigma^2 I_n) \), and a Gaussian design matrix \( X \in \mathbb{R}^{n \times p} \) with iid \( N(0, \Sigma) \) rows. We assume that the covariance matrix \( \Sigma \) is known and invertible.

This section explains how to construct an estimate of a linear contrast

\[ \theta = \langle a_0, \beta \rangle \]  

(3.57)

from an initial estimator \( \hat{\beta} \). Here and in the sequel, \( \langle \cdot, \cdot \rangle \) denotes the scalar product in \( \mathbb{R}^n \). Define

\[ u_0 = \Sigma^{-1}a_0/\langle a_0, \Sigma^{-1}a_0 \rangle, \quad z_0 = X u_0, \quad Q_0 = I_{p \times p} - u_0 a_0^\top \]  

(3.58)

and assume for simplicity that \( a_0 \) is normalized such that

\[ \langle a_0, \Sigma^{-1}a_0 \rangle = 1. \]

By definition of \( u_0, z_0 \sim N(0, I_n) \) and \( z_0 \) is independent of \( XQ_0 \).

We assume throughout this section that we are given an initial estimator \( \hat{\beta} \). Since \( X = z_0 a_0^\top + XQ_0 \) and the two random vectors \( z_0, XQ_0 \) are independent, we view \( \hat{\beta} \) as a function with three arguments \( \hat{\beta} = \beta(y, z_0, XQ_0) \) and we assume that the partial derivatives \( (\partial/\partial y) \hat{\beta} \) and \( (\partial/\partial z_0) \hat{\beta} \) exist almost everywhere.

The estimator \( \hat{\beta} \) provides an initial estimate of the unknown parameter \( \theta \) (3.57) by the plug-in \( \langle a_0, \hat{\beta} \rangle \). However, this estimator may be biased, and a first attempt to fix the bias is the following one-step MLE correction in the direction given by the one dimensional model \( \{ \hat{\beta} + tu_0, t \in \mathbb{R} \} \),

\[ \langle a_0, \hat{\beta} \rangle + \frac{\langle z_0, y - X\hat{\beta} \rangle}{\| z_0 \|^2}. \]  

(3.59)

Variants of the above de-biasing scheme have been considered in [Zha11, ZZ14, BCH14, Büh13, VdGBRD14, JM14, JM18], among others. We multiply by \( \| z_0 \|^2 \) to avoid random denominators; the random variables \( \| z_0 \|^2 \) is chi-square with \( n \) degrees of freedom, equal to \( n + O(\sqrt{n}) \) with overwhelming probability so that \( \| z_0 \|^2 \approx n \) describes the number of observations.

When constructing the estimator (3.59) above by the one-step MLE correction, the statistician hopes that the quantity

\[ \| z_0 \|^2 \langle a_0, \hat{\beta} - \beta \rangle + \langle z_0, y - X\hat{\beta} \rangle \]  

(3.60)

is asymptotically standard normal; this is the ideal result to construct confidence intervals for the unknown parameter (3.57) at the \( \sqrt{n} \)-adjusted rate.
By simple algebra we have

\[(3.61) \quad \|z_0\|^2 (a_0, \hat{\beta} - \beta) + (z_0, y - X\hat{\beta}) = z_0^\top \varepsilon - z_0^\top XQ_0 (\hat{\beta} - \beta).\]

The random variable \(z_0^\top \varepsilon\) in the right-hand side is mean-zero and \(z_0^\top \varepsilon/\sigma/\sqrt{n}\) is asymptotically standard normal. It remains to understand the bias term \(z_0^\top XQ_0 (\hat{\beta} - \beta)\). For the derivation below, we will argue conditionally on \((\varepsilon, XQ_0)\) and define \(f: \mathbb{R}^n \rightarrow \mathbb{R}^n\) by

\[f(z_0) = XQ_0 (\hat{\beta} - \beta).\]

The quantity \(f(z_0)\) is still biased and Stein’s formula lets us quantify the remaining bias in (3.61) exactly as follows

\[E\left[z_0^\top XQ_0 (\hat{\beta} - \beta) \mid XQ_0, \varepsilon\right] = E\left[z_0^\top f(z_0) \mid XQ_0, \varepsilon\right] = E\left[\text{div } f(z_0) \mid XQ_0, \varepsilon\right].\]

The partial derivatives \(\partial f_i / \partial z_{0i}\) where \(f_i\) is the \(i\)-th coordinate of \(f\) can be computed by the chain rule

\[\frac{\partial f_i}{\partial z_{0i}} = e_i^\top XQ_0 \left[\langle a_0, \beta \rangle \frac{\partial \hat{\beta}}{\partial y_i} + \frac{\partial \hat{\beta}}{\partial z_{0i}}\right].\]

Hence, the divergence of \(f\), which quantifies the remaining bias in (3.61) is

\[\text{div } f = \langle a_0, \beta - \hat{\beta} \rangle \hat{\nu} + \hat{B},\]

where

\[\hat{\nu} = \text{trace} \left[ XQ_0 \frac{\partial \hat{\beta}}{\partial y}\right], \quad \hat{B} = \text{trace} \left[ XQ_0 \frac{\partial \hat{\beta}}{\partial z_0}\right].\]

It will be convenient to write \(\text{div } f\) instead as

\[\text{div } f = \langle a_0, \beta - \hat{\beta} \rangle \hat{\nu} + \hat{B}, \quad \text{where } \hat{A} = \hat{B} + \langle a_0, \hat{\beta} \rangle \hat{\nu}.\]

The quantities \(\hat{\nu}, \hat{A}\) and \(\hat{B}\) above can be constructed from the observed data since they only depend on \(X, Q_0, y\) and the derivatives of \(\hat{\beta}\). However, the quantity \(\langle a_0, \beta \rangle\) is unknown; it is the parameter of interest that we wish to estimate. This motivates the estimator of \(\theta = \langle a_0, \beta \rangle\) defined by

\[\hat{\theta} = \langle a_0, \hat{\beta} \rangle + \frac{z_0^\top (y - X\hat{\beta}) + \hat{A}}{\|z_0\|^2 - \hat{\nu}}\]

with \(\hat{\nu}\) as in (3.62) and (3.63). This estimator \(\hat{\theta}\) is constructed so that the random variable

\[\left(\|z_0\|^2 - \hat{\nu}\right)(\hat{\theta} - \theta) - z_0^\top \varepsilon = \hat{A} + \hat{\nu}(a_0, \beta - \hat{\beta}) - z_0^\top f(z_0)\]

is exactly mean-zero by the first-order Stein’s formula (1.1). Furthermore, the variance of this random variable can be expressed exactly in terms of the
derivatives of \( f \) thanks to the Second Order Stein formula (2.3). Similarly, the above equality can be rewritten as

\[
(\|z_0\|^2 - \hat{\nu})(\hat{\theta} - \theta) = \text{div} f(z_0) - z_0^\top (f(z_0) - \varepsilon),
\]

which is equal to \( \text{div} g(z_0) - z_0^\top g(z_0) \) for \( g(x) = f(x) - \varepsilon \) since \( f \) and \( g \) have the same divergence. Hence the random variable (3.66) is exactly mean zero by the first-order Stein’s formula, and the Second Order Stein formula (2.3) provides an exact identity for its variance. We gather the above derivation in the following theorem.

**Theorem 3.15.** Let \( \hat{\beta} \) be an estimator such that, if we write it as a function \( \hat{\beta}(y, z_0, XQ_0) \), all partial derivatives of the function \( XQ_0\hat{\beta} \) with respect to \( y \) and \( z_0 \) exist and are in \( L_2 \). Define the estimator \( \hat{\theta} \) of \( \theta = (a_0, \beta) \) by (3.64), with \( \hat{\nu} \) and \( \hat{A} \) as in (3.62) and (3.63). Then the random variable

\[
\frac{(\|z_0\|^2 - \hat{\nu})(\hat{\theta} - \theta)}{\sigma\sqrt{n}} - \frac{z_0^\top \varepsilon}{\sigma\sqrt{n}}
\]

is exactly mean-zero and its variance is exactly equal to

\[
\frac{1}{n \sigma^2} \left( \mathbb{E} \left[ \|XQ_0(\hat{\beta} - \beta)\|^2 \right] + \mathbb{E} \left[ \text{trace}(\nabla f(z_0))^2 \right] \right)
\]

where \( f(z_0) = XQ_0(\hat{\beta} - \beta) \). Furthermore, the random variable \((\|z_0\|^2 - \hat{\nu})(\hat{\theta} - \theta)\) is also mean-zero with variance equal to

\[
\mathbb{E} \left[ \|X(\hat{\beta} - \beta) - y - z_0a_0^\top(\hat{\beta} - \beta)\|^2 + \text{trace}(\nabla f(z_0))^2 \right].
\]

Theorem 3.15 is a direct consequence of the Second Order Stein formula (2.3) and the analysis summarized in (3.65).

The random variable \( z_0^\top \varepsilon/(\sigma\sqrt{n}) \) is asymptotically standard normal. The first claim of the above result implies that \((\|z_0\|^2 - \hat{\nu})(\hat{\theta} - \theta))/\sigma\sqrt{n} \) is also asymptotically normal if (3.68) converges to 0 as \( n \to +\infty \). This provides a general strategy to derive asymptotic normality results; however the calculation of the gradients of \( \beta \) and \( f \) has to be carried out on case-by-case basis which is outside of the scope of the present paper.

The above construction provides a general scheme to de-bias an initial estimator \( \hat{\beta} \) for the estimation of a linear contrast \( \theta = (a_0, \beta) \) when the covariance matrix \( \Sigma \) is known because \((\|z_0\|^2 - \hat{\nu})(\hat{\theta} - \theta)\) is mean-zero and its variance is exactly given by (3.69). Notably, both \((\|z_0\|^2 - \hat{\nu})(\hat{\theta} - \theta)\) and the quantity inside the expectation in (3.69) only depends on the unknown parameter of interest \( \theta = a_0^\top \beta \) and known observable quantities \( a_0^\top \hat{\beta}, \hat{A}, \hat{\nu}, \hat{\beta} \) and its derivatives. One may consider the z-score \((\|z_0\|^2 - \hat{\nu})(\hat{\theta} - \theta)/V^*(\theta)^{1/2} \) where \( V^*(\theta) \) is the quantity inside the expectation in (3.69). First and Second Order Stein formulae provide this z-score as the starting point to de-bias the general estimator \( \hat{\beta} \) and normalize its variance, as soon as the partial derivatives
of $\hat{\beta}$ exist. Studying the asymptotic distribution of this z-score requires tools beyond the scope of the present work and will be the subject of a forthcoming paper.

A notable feature of the above result is the random variable $\hat{\nu}$ whose role is to adjust multiplicatively the random variable $(\hat{\theta} - \theta)$ so that $(\|z_0\| - \hat{\nu})(\hat{\theta} - \theta)$ is exactly mean-zero. This adjustment accounts for the degrees-of-freedom of the initial estimator $\hat{\beta}$. We refer to our concurrent paper [BZ18] for theory of degrees-of-freedom adjustment in semi-parametric inference about a preconceived one-dimensional parameter $\theta = (a_0, \beta)$.

### 3.7. Monte Carlo approximation of divergence

The Second Order Stein formula and the techniques presented in this paper also suggest a Monte Carlo method to approximate the divergence in the general case.

Suppose we are interested in the approximation of $\text{div} f(y)$ at the currently observed vector $y$. Assume that the function $f(\cdot)$ is 1-Lipschitz and its value can be quickly computed for small perturbations of $y$, say, $f(y + az)$ for small $az$.

For example, when $f(y) = X\hat{\beta}$ in the linear model with a convex regularized least-squares estimator $\hat{\beta}$, the 1-Lipschitz condition holds automatically [BT17] as discussed in Remark 3.3, and if $\hat{\beta}(y)$ has already been computed by an iterative algorithm, the computation of $\hat{\beta}(y + az)$ would typically be fast as one can use $\hat{\beta}(y)$ as a starting point ("warm start") to compute $\hat{\beta}(y + az)$. Next, with the 1-Lipschitz function $h(z) = a^{-1}(f(y + az) - f(y))$ and $z \sim N(0, I_n)$ independent of $y$, if $E_z$ denotes the expectation with respect to $z$ conditionally on $y$, we have by the Gaussian Poincaré inequality that

$$E_z[(z^\top h(z) - D_0)^2] \leq E_z[\|h(z) + \nabla h(z)\|^2] \leq 4n$$

with $D_0 = E_z \text{div} h(z) = \int_{\mathbb{R}^n} e^{-\|z\|^2/2} \text{div} f(y + ax) dx$. Hence if we compute $f(y + az_j)$ at $m$ independent Gaussian perturbations $z_1, ..., z_m \sim N(0, I_n)$, inequality

$$E \left[ \left( \frac{1}{m} \sum_{j=1}^m z_j^\top h(z_j) - D_0 \right)^2 \bigg| y \right] \leq \frac{4n}{m}$$

holds. Here the function $y \rightarrow \text{div}(y)$ is locally integrable and almost surely bounded by $n$ thanks to the Lipschitzness of $f$. For almost every $y$, $y$ is a Lebesgues point of $\text{div} f$ so that $D_0 \rightarrow \text{div}(y)$ as $a \rightarrow 0$ by the Lebesgues differentiation theorem. Hence $D_0 \approx \text{div} f(y)$ for small enough $a > 0$ and $\frac{1}{m} \sum_{j=1}^m z_j^\top h(z_j)$ provides a useful approximation of the divergence thanks to the above conditional variance bound. For large $m$, more precise results can be obtained by the central limit theorem. Note that by the Second Order Stein formula, $\frac{1}{m} \sum_{j=1}^m z_j^\top h(z_j)$ is also close to the empirical average $D^{(m)} = ...
$\frac{1}{m} \sum_{j=1}^{m} \text{div} f(y + az_j)$ thanks to

$$
\mathbb{E} \left[ \left( \frac{1}{m} \sum_{j=1}^{m} z_j h(z_j) - \hat{D}(\mu) \right)^2 \right] = \frac{1}{m} \mathbb{E} \left[ \|h(z_1)\|^2 + \text{trace} \{ \nabla h(z_1) \} \right] \leq \frac{2n}{m}.
$$

We apply this probabilistic procedure to the Elastic-Net and Singular Value Thresholding (SVT) [CSLT13] for which explicit formulae for $\hat{df} = \text{trace} \{ \nabla f(y) \}$ are available.

Indeed, [CSLT13, Equation (1.8)] provides an explicit formula for the degrees-of-freedom of SVT with tuning parameter $\lambda$: If $\hat{B}$ soft-thresholds the singular values of an observed matrix $Y \in \mathbb{R}^{m \times n}$ with tuning parameter $\lambda$, the divergence of $\hat{B}$ with respect to $Y$ is given by

$$
\hat{df} = \sum_{i=1}^{q \wedge n} \left\{ I(\sigma_i > \lambda) + |q - n| (1 - \lambda/\sigma_i)_+ \right\} + 2 \sum_{i=1}^{q \wedge n} \sum_{j=1, j \neq i}^{q \wedge n} \frac{\sigma_i (\sigma_i - \lambda)_+}{\sigma_i^2 - \sigma_j^2} \sigma_i \hat{Z}_j,
$$

where $\sigma_1, \ldots, \sigma_{n \wedge q}$ are the singular values of $Y$. We then compare on simulated data this exact formula to the above random approximation scheme. For $n = 100, q = 101, \lambda = 10.0$, with $Y$ being the sum of standard normal noise plus a ground-truth rank-10 matrix, we apply the above algorithm with $m$ perturbations $(Y + a Z_j)_{j=1, \ldots, m}$ for various values of $m$ and compute $\hat{df}_{\text{approx}} = \frac{1}{m} \sum_{j=1}^{m} \text{trace} \{ \hat{Z}_j h(\hat{Z}_j) \}$ where $h(\hat{Z}_j) = a^{-1} (\hat{B}(Y + a Z_j) - \hat{B}(Y))$ with $a = 0.0001$ as explained above. The results are in Figure 1.

In the case of the Elastic-Net with $\ell_1$ parameter $\lambda > 0$ and $\ell_2$ parameter $\gamma > 0$, we draw a similar experiment with the exact formula for degrees-of-freedom being given by $\hat{df} = \text{trace} \{ X_S (X_S^\top X_S + \nu \gamma)^{-1} X_S^\top \}$ as in Section 3.5.3. With $n = 500, p = 400$, and again $a = 0.001$, $X$ having independent symmetric ±1, $\lambda = 0.8 \sqrt{4 \log(p)/n}$, $\gamma = 0.2 \sqrt{4 \log(p)/n}$, we obtain the standard errors and boxplots in Figure 2.

The experiments show that the above approximation scheme provides good approximations in these special cases where exact formula are available. Hence it could also be useful for estimators where no exact formula is available for the divergence.

**Appendix A: Non-smooth functions**

**Proof of Theorem 2.1 (ii) for Lipschitz functions.** If $f$ is Lipschitz, then each component $f_i$ of $f$ is also Lipschitz. Hence $f_i$ belongs to the space $W^{1,2}(\gamma_n)$ defined above (2.2) and the weak gradient of $f_i$ is equal almost everywhere to its gradient in the sense of Frechet differentiability (cf., e.g. [Eva97, Theorem 4-6 pp 279-281]). Thus (ii) is a consequence of (iii). \( \square \)

**Proof of Theorem 2.1 (iii) for $f_i \in W^{1,2}(\gamma_n)$.** Since $W^{1,2}(\gamma_n)$ is the completion with respect to the norm (2.2) of the space $C_0^\infty(\mathbb{R}^n)$ of smooth functions with compact support, for each coordinate $i = 1, \ldots, n$ there exists a sequence $(g_{i,q})_{q \geq 1}$
of $C_0^\infty(\mathbb{R}^n)$ functions with $\max_{i=1,\ldots,n} E[(f_i - g_{i,q})^2 + \|\nabla f_i - \nabla g_{i,q}\|^2] \to 0$ as $q \to +\infty$. Define $g_q : \mathbb{R}^n \to \mathbb{R}^n$ as the function with components $g_{1,q}, \ldots, g_{n,q}$. By considering a subsequence, we may assume that for all $q \geq 1$,

$$E\left[\|g_q(z) - f(z)\|^2\right] + E\left[\|\nabla g_q(z) - \nabla f(z)\|^2\right] \leq 2^{-q-2}$$

which implies that $g_q \to f$ and $\nabla g_q \to \nabla f$ pointwise almost surely by the Borel-Cantelli lemma. Let $X_q = z^T g_q(z) - \text{div} \, g_q(z)$ and $X = z^T f(z) - \text{div} \, f(z)$. Then $X_q \to X$ almost surely. The triangle inequality and Theorem 2.1 (i) applied to $g_k - g_{k+1}$ yields

$$\{E[(X_q - X)^2]\}^{1/2} \leq \sum_{k=q}^{\infty} \{E[(X_k - X_{k+1})^2]\}^{1/2} \leq \sum_{k=q}^{\infty} \{E[\|g_k(z) - g_{k+1}(z)\|^2] + E[\|\nabla g_k(z) - \nabla g_{k+1}(z)\|^2]\}^{1/2} \leq \sum_{k=q}^{\infty} 2^{-k/2} \to 0.$$

Hence, with another application of Theorem 2.1(i),

$$E\left[(z^T f(z) - \text{div} \, f(z))^2\right] = \lim_{q \to \infty} E\left[(z^T g_q(z) - \text{div} \, g_q(z))^2\right] = \lim_{q \to \infty} E[\|g_q(z)\|^2 + \text{trace} \left((\nabla g_q)^2(z)\right)] = E[\|f(z)\|^2 + \text{trace} \left((\nabla f)^2(z)\right)].$$

For the first and last equality, we use the fact that if two sequences $(Z_q)_{q \geq 1}$ and $(Y_q)_{q \geq 1}$ and two random variables $Y_{\infty}, Z_{\infty}$ are such that $E[(Y_q - Y_{\infty})^2] \to 0$ and $E[(Z_q - Z_{\infty})^2] \to 0$ as $q \to +\infty$ then $E[Y_q^2] \to E[Y_{\infty}^2]$ and $E[Y_q Z_q] \to E[Y_{\infty} Z_{\infty}]$. This completes the proof. \qed

**Appendix B: Proof of consistency**

**Proof of Theorem 3.2.** (i) Since $E[\hat{\mu}] = E[\|\hat{\mu} - \mu\|^2],

$$E[\hat{R}'_{\text{SURE}}] = E[2\sigma^2\|y - \hat{\mu}\|^2 + 2\sigma^2\|\hat{\mu} - \mu\|^2] \geq \sigma^2 E[\|\varepsilon\|^2] = \sigma^4 n.$$

(ii) As $((\hat{\mu})_+^{1/2} - \|\hat{\mu} - \mu\|)_+^{1/2} \leq |\hat{\mu} - \mu|\|\hat{\mu} - \mu\|^2$, by the triangle inequality

$$E\left[((\hat{\mu})_+^{1/2} - E[\|\hat{\mu} - \mu\|^2])^{1/2}\right] \leq E\left[\left((\hat{\mu})_+^{1/2} - E[\|\hat{\mu} - \mu\|^2]\right)^{4/2}\right]^{1/4}.$$
Proof of Remark 3.3.  The claim that \( \hat{\mu} = X \hat{\beta}(y) \) is 1-Lipschitz is proved in [BT17, Proposition 3]. The symmetry and positivity of \( \nabla \hat{\mu} \) is proved in [BZ19, Proposition J.1] with the argument outlined here: \( \hat{\mu}(y) \in \partial u(y) \) where the function \( u(y) = \|y\|^2/2 - \|X \hat{\beta}(y) - y\|^2/2 - g(\hat{\beta}(y)) \) is convex, Alexandrov’s theorem on the almost sure second order differentiability of convex functions given for instance in [NP06, Theorem D.2.1] grants that the Hessian of \( u \) is almost surely symmetric positive semi-definite, and the Hessian of \( u \) equals \( \nabla \hat{\mu}(y) \) almost surely. \( \square \)
Appendix C: Proofs: Confidence regions with SURE

Proof of Theorem 3.4 and Corollary 3.5. Assume $\sigma = 1$ without loss of generality. As $f(y) = \hat{\mu} - y = (\hat{\mu} - \mu) = \varepsilon$,

$$\text{SURE} - \|\mu - \hat{\mu}\|^2 = \|\hat{\mu} - y\|^2 - \|\mu - \hat{\mu}\|^2 + 2\text{div}(\hat{\mu} - y) + n$$

so that (3.18) is a direct consequence of Theorem 2.1. By Markov’s inequality,

$$\mathbb{P}\left\{\|\varepsilon^T(\hat{\mu} - \mu) - \text{div}(\hat{\mu} - \mu)\| \geq v_0\sqrt{n/2}\right\} \leq \mathbb{E}[\|\hat{\mu} - \mu\|^2 + \text{trace}((\nabla \hat{\mu}(y))^2)]/(v_0^2n/2) \leq \epsilon_n.$$

The conclusion follows from the definition of $v_n$ and the union bound.

Corollary 3.5 follows from Theorem 3.4 with $v_0^2 = 2\gamma_n^1/\epsilon$, $\epsilon_n = \gamma_n^1/2$ and the continuous mapping theorem.

Proof of Theorem 3.6. Assume $\sigma = 1$ without loss of generality. Set $\hat{d}\hat{f} = \text{trace}(\nabla \hat{\mu})$, $h = \hat{\mu} - \mu$ and $W = \text{SURE} - \mathbb{E}[\|\hat{\mu} - \mu\|^2] - \|\varepsilon\|^2 + n$. As $W$ is of the form (2.10) with $f(\varepsilon) = -2h$ and $g(\varepsilon) = \mathbb{E}[\|h\|^2] - \|h\|^2$,

$$\text{Var}(W) \leq \mathbb{E}[\|\hat{\mu} - \mu\|^2 + \text{trace}((\nabla \hat{\mu}^2))] \leq \mathbb{E}[2\|h\|^2 + 4\text{trace}((\nabla \hat{\mu}^2))] \leq 4\mathbb{E}[\text{SURE} + \hat{d}\hat{f}].$$

by (2.12). This gives (3.22). Let $X_n = |W|/\mathbb{E}[W^2]^{1/2}$. We have

\begin{equation}
|W| \leq 2X_n(\mathbb{E}[\text{SURE} + \hat{d}\hat{f}])^{1/2}.
\end{equation}

As $\text{SURE} + \hat{d}\hat{f}$ is of form (2.10) with $f(\varepsilon) = \varepsilon - 3h$ and $g(\varepsilon) = -\varepsilon^T h - \|h\|^2$, (2.12) yields

$$\text{Var}(\text{SURE} + \hat{d}\hat{f}) \leq \mathbb{E}[\|\varepsilon - 2h + (\nabla \hat{\mu})(2h + \varepsilon)\|^2 + \text{trace}((I_n - 3\nabla \hat{\mu}^2))]$$

Using $\text{trace}(\nabla \hat{\mu}^2) \leq \hat{d}\hat{f}$, the second term is bounded by $n - 6d\hat{f} + 9d\hat{f} = n + 3d\hat{f}$. Since $(2h + \varepsilon)(\nabla \hat{\mu})^2(2h + \varepsilon) \leq (2h + \varepsilon)(\nabla \hat{\mu})(2h + \varepsilon)$, expanding the square yields

\begin{align*}
\text{Var}(\text{SURE} + \hat{d}\hat{f}) &\leq \mathbb{E}[\|\varepsilon - 2h\|^2 + (2h + \varepsilon)(\nabla \hat{\mu})(2h + \varepsilon) + 2(\varepsilon - 2h)^T(\nabla \hat{\mu})(2h + \varepsilon)] + \mathbb{E}[n + 3d\hat{f}] \\
&= \mathbb{E}[n + 3d\hat{f} + \|\varepsilon - 2h\|^2 + 4\varepsilon^T(\nabla \hat{\mu})\|\varepsilon\| - \mathbb{E}[(\varepsilon - 2h)^T(\nabla \hat{\mu})(\varepsilon - 2h)]] \\
&\leq \mathbb{E}[4\text{SURE} + (6n - \hat{d}\hat{f})]
\end{align*}

where the last inequality follows from $\varepsilon^T(\nabla \hat{\mu})\varepsilon \leq \|\varepsilon\|^2$ and Stein’s formulae $\mathbb{E}[-4\varepsilon^T h] = \mathbb{E}[-4d\hat{f}]$ and $\mathbb{E}[\|h\|^2] = \mathbb{E}[\text{SURE}]$. Hence there exists a random
variable $Y_n \geq 0$ with $\mathbb{E}[Y_n^2] \leq 1$ such that almost surely $\mathbb{E}[\tilde{\text{SURE}} + \hat{f}] \leq \tilde{\text{SURE}} + \hat{f} + 2Y_n \mathbb{E}[\tilde{\text{SURE}} + \hat{f}]^{1/2} + Y_n \sqrt{6n}$. By completing the square,

\[(C.2) \quad (\mathbb{E}[\tilde{\text{SURE}} + \hat{f}]^{1/2} - Y_n)^2 \leq \tilde{\text{SURE}} + \hat{f} + Y_n^2 + Y_n \sqrt{6n}.\]

Combining (C.1) and (C.2) above we get almost surely

\[|W| \leq 2X_n \left[ (\tilde{\text{SURE}} + \hat{f})^{1/2} + 2Y_n + \sqrt{Y_n}(6n)^{1/4} \right]\]

which is equivalent to (3.23). As $X_n \leq 1/\sqrt{\beta_1}$ and $Y_n \leq 1/\sqrt{\beta_2}$ with probability at least probability $1 - \beta_1 - \beta_2$, the conclusions follow.

For the estimation of $\|\hat{\mu} - \mu\|^2$, we set $W = \tilde{\text{SURE}} - \|\hat{\mu} - \mu\|^2 - \|\varepsilon\|^2 + n$ with $\mathbb{E}[W^2] \leq 4\mathbb{E}[\tilde{\text{SURE}} + \hat{f}]$ in virtue of $\text{trace}(\{\nabla \hat{\mu}\}) \leq \hat{f}$ by 1-Lipschitzness of $\hat{\mu}$ so that the upper bounds for $\mathbb{E}[\tilde{\text{SURE}} + \hat{f}]$ still apply. □

D. Proofs of Theorem 3.7, Proposition 3.8 and (3.32)

The proof of Theorem 3.7 requires the following lemma.

**Lemma D.1.** Consider the sequence model $y = \mu + \varepsilon$ with $\varepsilon \sim N(0, \sigma^2 I_n)$. Let $\hat{\mu}^{(1)}, \hat{\mu}^{(2)}$ be two estimators that are $L$-Lipschitz functions of $y$ and let $f(y) = \hat{\mu}^{(2)} - \hat{\mu}^{(1)}$. Let $\hat{\mu}$ be the estimator among $\{\hat{\mu}^{(1)}, \hat{\mu}^{(2)}\}$ with the smallest $\tilde{\text{SURE}}$. Then either

\[\mathbb{E}[\Delta^2] \leq 8\sigma^4 \mathbb{E}[\text{trace}(\{\nabla f(y)\})^2] \quad \text{or} \quad \mathbb{E}[\Delta^2] \leq 8(\sqrt{2L} + 1)^2\]

holds, where $\Delta = \|\hat{\mu} - \mu\| - \min_{j=1,2} \|\hat{\mu}^{(j)} - \mu\|$.

**Proof of Lemma D.1.** Let $\xi = \|\hat{\mu}^{(1)} - \mu\|^2 - \|\hat{\mu}^{(2)} - \mu\|^2 - \tilde{\text{SURE}}^{(1)} + \tilde{\text{SURE}}^{(2)} = 2 \text{div} f(y) - 2\varepsilon^\top f(y)$. By definitions of $\hat{\mu}$ and $\Delta$,

\[|\xi| \geq \|\hat{\mu} - \mu\|^2 - \min_{j=1,2} \|\hat{\mu}^{(j)} - \mu\|^2 \]

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

\[\geq \|f(y)\| \Delta \vee \Delta^2.\]

If $\sigma^2 \mathbb{E}[\text{trace}(\{\nabla f(y)\})^2] \geq \mathbb{E}[f(y)^2]$ then $\mathbb{E}[\Delta^4] \leq \mathbb{E}[\xi^2]$ and the identity (2.7) for $\mathbb{E}[\xi^2]/4$ yields the bound on $\mathbb{E}[\Delta^4]$.

If now $\sigma^2 \mathbb{E}[\text{trace}(\{\nabla f(y)\})^2] \leq \mathbb{E}[f(y)^2]$, as $y \rightarrow \|f(y)\|$ is $2L$-Lipschitz

\[\mathbb{E}[\|f(y)\|^2] \mathbb{E}[\Delta^2] \leq \mathbb{E}[\|f(y)\|^2 \Delta^2] + \{\text{Var}(\|f(y)\|^2) \mathbb{E}[\Delta^4]\}^{1/2} \]

\[\leq \mathbb{E}[\xi^2] + \{\text{Var}(\|f(y)\|^2) \mathbb{E}[\xi^2]\}^{1/2} \leq 8\sigma^2 \mathbb{E}[\|f(y)\|^2] \mathbb{E}[\|f(y)\|^2] + \sqrt{(4L)^2 8 \sigma^2 \mathbb{E}[\|f(y)\|^2]},\]

by the Cauchy-Schwarz inequality for the first inequality and the Gaussian Poincaré inequality $\text{Var}[\|f(y)\|^2] \leq \mathbb{E}[\|2\nabla f(y)\|^2 f(y)] \leq (4L)^2 \mathbb{E}[\|f(y)\|^2]$ for the second. Hence $\mathbb{E}[\Delta^2] \leq 8(\sqrt{2L} + 1)^2 \sigma^2$. □
Proof of Theorem 3.7. Let \( j_0 = \arg \min_{j=1, \ldots, m} \mathbb{E}[\|\hat{\mu}^{(j)} - \mu\|] \). For \( k \in [m] \), let
\[
\Delta_k = I_k (\|\hat{\mu}^{(k)} - \mu\| - \|\hat{\mu}^{(j_0)} - \mu\|)_+, 
\]
where \( I_k \) is the indicator of the event that the \textit{SURE} of \( \hat{\mu}^{(k)} \) is smaller than the \textit{SURE} of \( \hat{\mu}^{(j_0)} \). Then by Lemma D.1 we have \( \mathbb{E}[A_k] \leq 1 \) with
\[
A_k = \min \{ \Delta_k^2 / (8\sigma^4 s^*), \Delta_k^2 / (8\sigma^2 (\sqrt{2L} + 1)) \}
\]
and \( X = m^{-1} \max_{k \in [m]} A_k \) has also \( \mathbb{E}[X] \leq 1 \). Then almost surely,
\[
(D.1) \quad \|\hat{\mu} - \mu\| - \|\hat{\mu}^{(j_0)} - \mu\| \leq \Delta_k \leq \sigma \max \{ (8s^* mX)^{1/4}, (8(\sqrt{2L} + 1)mX)^{1/2} \}
\]
so that \( \mathbb{P}(X > 1/\alpha) \leq \alpha \) yields (i).

(ii) Set \( W_k = (\|\hat{\mu}^{(j_0)} - \mu\| - \|\hat{\mu}^{(k)} - \mu\|)_+ \). For each \( k \in [m] \), the function \( y \rightarrow \|\hat{\mu}^{(j_0)} - \mu\| - \|\hat{\mu}^{(k)} - \mu\| \) is \( 2L \)-Lipschitz with negative expectation so that \( \mathbb{P}(W_k > 2\sigma \sqrt{2x}) \leq e^{-x} \) for all \( x > 0 \) by Gaussian concentration and \( \mathbb{P}(\max_{k \in [m]} W_k > 2\sigma \sqrt{2 \log(m/\delta)}) \leq \delta \) by the union bound.

(iii) is obtained using (D.1), \( \mathbb{E}[X] \leq 1 \) and \( \mathbb{E}[\max_{k \in [m]} W_k^2] \leq 8L^2\sigma^2 \log(em) \) by integration.

(iv) For (3.29), let \( k_0 = \arg \min_{j \in [m]} \mathbb{E}[\|\hat{\mu}^{(j)} - \mu\|^2] \). For all \( j, k \in [m] \) we have for \( \xi_{j,k} = \|\hat{\mu}^{(k)} - \mu\|^2 - \text{SURE}^{(k)} - \|\hat{\mu}^{(j)} - \mu\|^2 + \text{SURE}^{(j)} \) that
\[
\mathbb{E}[\xi_{j,k}^2] = 4\mathbb{E}[\sigma^2 \|\hat{\mu}^{(j)} - \hat{\mu}^{(k)}\|^2 + 4\sigma^4 \text{trace}(\{\nabla\hat{\mu}^{(k)} - \nabla\hat{\mu}^{(j)}\|^2)] 
\leq 16L^2\sigma^4 n + 16L^2\sigma^4 n = 32L^2\sigma^4 n
\]
by assumption. Since \( G = \max_{k \in [m]} \xi_{k_0,k}^2 / (32L^2\sigma^4 mn) \) has \( \mathbb{E}[G] \leq 1 \) and \( \|\hat{\mu} - \mu\|^2 - \|\hat{\mu}^{(k_0)} - \mu\|^2 \leq (32Gmn)^{1/2} \) holds a.s., we get (3.29).

\[
\square
\]

Proof of Proposition 3.8. Let \( v \in \mathbb{R}^n \) with \( \|v\|^2 = \sigma^2 \sqrt{n} \). Choose
\[
\mu = 0, \quad \hat{\mu}^{(1)}(y) = 0, \quad \hat{\mu}^{(2)}(y) = v + G(y)
\]
where \( G : \mathbb{R}^n \rightarrow \mathbb{R}^n \) with \( G(y)_i = g(y_i) \) and \( g \) is defined as the only function that is \( 2^n+1 \sigma \) periodic, symmetric \( (g(-u) = g(u)) \) and with \( g(u) = \sigma (\frac{u}{\sigma} \wedge (2^n - \frac{u}{\sigma})) \) on \([0, 2^n\sigma] \). Observe that \( g \) and \( G \) are both \( 1 \)-Lipschitz. Furthermore, \( \mathbb{P}(g(y)_i = \pm 1) = 1/2 \) by symmetry of \( g \) and \( \text{div} \ G(y) = \sum_{i=1}^n r_i \) where \( (r_1, \ldots, r_n) \) are iid with \( \mathbb{P}(r_i = \pm 1) = 1/2 \). Since \( \hat{\mu}^{(1)} \) is the oracle, i.e., it has smaller risk than \( \hat{\mu}^{(2)} \), we now study the event \( \Omega = \{ \text{SURE}^{(2)} < \text{SURE}^{(1)} \} \) in which \( \hat{\mu} \) selects the worse estimator. Event \( \Omega \) can be rewritten \( \{ \|v + G(y)\|^2 - 2\sigma^2 (v + G(y)) + 2\sigma^2 \text{div} G(y) \leq 0 \} \). We have \( \mathbb{P}(\text{div} G(y) \leq -\sqrt{n}) \geq C_0 > 0 \) by the reverse of Hoeffding inequality given in [MV08, Theorem 7.3.2], while \( \|v + G(y)\|^2 - 2\epsilon \sigma^2 (v + G(y)) \leq \sigma^2 \sqrt{n} (1 + o_p(1)) \) since \( \|v\|^2 = \sigma^2 \sqrt{n}, |G| \leq o(2^{-n}) \) and \( \epsilon \sigma \|v\| = O_p(\sigma \|v\|) \). This proves that \( \mathbb{P}(\Omega) \geq C_0 > 0 \) for instance with \( C_3 = C_0/2 \) and any \( n \geq C_1 \) for large enough \( C_1 \). On \( \Omega \), we have \( \hat{\mu} = \hat{\mu}^{(2)} \) as well as
\[
\|\hat{\mu} - \mu\| - \|\hat{\mu}^{(1)} - \mu\| = \|\hat{\mu}^{(2)} - \mu\| = \|v + G(y)\| \geq C_2 \sigma n^{1/4}. 
\]
\[
\square
\]
Proof of (3.32) assuming $y \to \hat{\mu}^{(j)}(y)$ is $L$-Lipschitz for all $j$. Let $k \in [m]$ be fixed. Proposition 3.2 in [Bel18] states that $\mu_Q$ satisfies
\[
\|\hat{\mu}_Q - \mu\|^2 - \|\hat{\mu}_Q^{(j_0)} - \mu\|^2 
\leq \max_{k \in [m]} 2\{\varepsilon^T (\hat{\mu}^{(k)} - \hat{\mu}^{(j_0)}) - \sigma^2 \text{div}(\hat{\mu}^{(k)} - \hat{\mu}^{(j_0)}) - \|\hat{\mu}^{(j_0)} - \hat{\mu}^{(k)}\|^2 / 4\}.
\]

Let $W_{j_0,k}$ be the random variable inside the maximum, which is of the form (2.10) with $f(\varepsilon) = (\hat{\mu}^{(k)} - \hat{\mu}^{(j_0)})$ and $g(\varepsilon) = \|f(\varepsilon)\|^2 / 4$. Then $G = \max_{j \in [m]} (W_{j_0,k} - \mathbb{E}(W_{j_0,k}))^2 / (m \text{Var}(W_{j_0,k}))$ has $\mathbb{E}(G) \leq 1$ and $\text{Var}(W_{j_0,k}) \leq \sigma^2 \|((I_n - \frac{1}{2} \nabla f) f)\|^2 + \sigma^4 s^* \leq (1 + L)^2 \sigma^2 \mathbb{E}(\|\hat{\mu}^{(j_0)} - \hat{\mu}^{(k)}\|^2) + \sigma^4 s^* \text{ by (2.12)}$. Then almost surely
\[
W_{j_0,k} \leq \sqrt{Gm \text{Var}(W_{j,0,k})}^{1/2} - \mathbb{E}(\|\hat{\mu}^{(j_0)} - \hat{\mu}^{(k)}\|^2 / 4)
\leq \sigma^2 \sqrt{Gms^2} + (1 + L)^2 \mathbb{E}(\|\hat{\mu}^{(j_0)} - \hat{\mu}^{(k)}\|^2)^{1/2} - \mathbb{E}(\|\hat{\mu}^{(j_0)} - \hat{\mu}^{(k)}\|^2 / 4)
\leq \sigma^2 \sqrt{Gms^2} + (1 + L)^2 \sigma^2 G.
\]

The proof is complete using $\mathbb{E}(G) \leq 1$ and $\mathbb{E}(\|\hat{\mu}^{(j_0)} - \mu\|^2 - \min_{j \in [m]} \mathbb{E}(\|\hat{\mu}^{(j)} - \mu\|^2) \leq \sigma^2 L^2$ by definition of $j_0$ and $L$-Lipschitz of $\hat{\mu}^{(j_0)}$. \hfill \Box

E. Strictness of the KKT conditions

Proof of Proposition 3.9. Assume that $X_B$ has rank strictly less than $|B|$. Then there must exist some $j \in B$ and $A \subseteq B \setminus \{j\}$ with $x_j = \sum_{k \in A} \gamma_k x_k$ and rank($X_A$) = min(|A|, n). By the definition of $B$
\[
\lambda n \delta_j = x_j^T (y - X \hat{\beta}_{v_{\lambda\text{lasso}}}^A) = \lambda n \sum_{k \in A} \gamma_k \delta_k
\]
where $\delta_k = x_k^T (y - X \hat{\beta}_{v_{\lambda\text{lasso}}}^A) / (\lambda n) \in \{-1, 1\}$. This is impossible by Assumption 3.1 on $X$. Hence $X_B$ has rank $|B|$. For the uniqueness, consider two Lasso solutions $\hat{\beta}_{v_{\lambda\text{lasso}}}^A$ and $\hat{\beta}$ of (3.34). It is easily seen that $X \hat{\beta}_{v_{\lambda\text{lasso}}}^A = X \hat{\beta}$ by the strict convexity of the squared loss in $X \beta$ in (3.34); actually the function $y \to X \hat{\beta}_{\lambda\text{lasso}}^A$ is 1-Lipschitz (cf. for instance [BLT18]). Furthermore both $\hat{\beta}_{v_{\lambda\text{lasso}}}^A, \hat{\beta}$ must be supported on $B$. Hence $X_B(\hat{\beta}_{v_{\lambda\text{lasso}}}^A)_B = X_B \hat{\beta}_B$ which implies that $\hat{\beta}_B = (\hat{\beta}_{v_{\lambda\text{lasso}}}^A)_B$ because $X_B$ has rank $|B|$.

It remains to show that for any $j \notin \hat{S}$, the KKT conditions on coordinate $j$ holds strictly with probability one. As $X_B$ has rank $|B|$, it suffices to consider the case of $|\hat{S}| < n$. By the KKT conditions, $(\hat{\beta}_{v_{\lambda\text{lasso}}}^A)_j = (X_{\hat{S}}^T X_{\hat{S}})^{-1} (X_{\hat{S}}^T y - n \lambda sgn((\hat{\beta}_{\lambda\text{lasso}}^A)_j))$. As $\mathbb{P}(v^T y = c) = 0$ for all deterministic $v \neq 0$ and real $c$,
\[
\mathbb{E}\left(\mathbb{P}\left(\left\{ y - X_{\hat{S}}(X_{\hat{S}}^T X_{\hat{S}})^{-1}(X_{\hat{S}}^T y - n \lambda s) / n \right\} = \pm \lambda \right| X_{\hat{S}}\right)\right) = 0
\]
for all deterministic $\{S, j, u\}$ satisfying rank($X_S$) = $|S| < n$, rank($X_{S \cup \{j\}}$) = $|S| + 1$ and $u \in \{\pm 1\}^S$. Hence, $\mathbb{P}(|B| > |\hat{S}|) = 0$, which means that the KKT conditions of $\hat{\beta}_{v_{\lambda\text{lasso}}}^A$ must hold strictly with probability one. \hfill \Box
F. Proof: bound on the variance of $|\hat{S}|$

Proof of Theorem 3.11. Assume $\sigma = 1$ without loss of generality due to scale invariance. The first claim follows from (3.37) and the discussion leading to it, combined with Theorem 2.2. Next we first use the rough bounds $|\hat{S}| \leq n$ and $\|P_S \epsilon\| \leq \|\epsilon\|$ to obtain $\text{Var}[|\hat{S}|] \leq 2n$. For the right term of the minimum, for a fixed $A \subset [p]$, the random variable $\|P_A \epsilon\|^2$ has chi-squared distribution with at most $|A|$ degrees of freedom and a classical tail bound (cf. for instance [LM00, Lemma 1]) states that

$$\text{P}(\|P_A \epsilon\|^2 > 2|A| + 3x) \leq \text{P}(\|P_A \epsilon\|^2 > |A| + 2\sqrt{|A|} + 2x) \leq e^{-x}.$$ 

Consequently, by the union bound over all $(\binom{p}{m}) \leq (\frac{e\pi}{m})^m$ supports $A$ of size $m$, 

$$\text{P}\left(\max_{A \subset [p]} \|P_A \epsilon\|^2 > 2m + 3\left(m \log \left(\frac{ep}{m}\right) + x\right)\right) \leq e^{-x}.$$ 

By a second union bound over all possible support sizes $m = 1, ..., p$, 

$$\text{P}\left(\max_{A \subset [p]} \left\{\|P_A \epsilon\|^2 - 2|A| - 3\left(|A| \log \left(\frac{ep}{|A| \lor 1}\right)\right)\right\} > 3(\log p + x)\right) \leq e^{-x}.$$ 

Finally, let $X = (1/3) \max_{A \subset [p]} \{\|P_A \epsilon\|^2 - 2|A| - 3(|A| \log (\frac{ep}{|A|} + \log p))\}$ so that $\text{P}(X > x) \leq e^{-x}$ holds. The identity $\text{E}[\text{max}(X, 0)] = \int_0^\infty \text{P}(X > x) dx \leq 1$ yields 

$$\text{E}[\|P_S \epsilon\|^2] \leq 2\text{E}[|S|] + 3\text{E}\left[|S| \log \left(\frac{ep}{|S| \lor 1}\right)\right] + \log(ep) \leq 2\text{E}[|S|] + 4\text{E}\left[|S| \log \left(\frac{ep}{|S| \lor 1}\right)\right].$$ 

The proof is complete as the second inequality in (3.39) follows from the concavity of the function $x \rightarrow x \log(ep/(x \lor 1))$. 

G. Preliminaries for bounds on $\text{E}[\hat{S}]$

Lemma G.1. Let $Z$ be a standard normal random variable. Then,

$$\text{P}\left[Z > t\right] \leq \frac{e^{-t^2/2}}{(2\pi t^2 + 4)^{1/2}}, \quad \forall \ t \geq 0,$$

$$\text{E}\left[(|Z| - t)_+\right] \leq \frac{2e^{-t^2/2}}{(2\pi)^{1/2}(t^2 + 1)}, \quad \forall \ t \geq 0,$$

and

$$\text{E}\left[(|Z| - t)_+^2\right] \leq \frac{4e^{-t^2/2}}{(t^2 + 2)(2\pi t^2 + 4)^{1/2}}, \quad \forall \ t \geq 0.$$ 

(G.1)
Remark Compared with the usual tail probability bounds for standard Gaussian, the upper bounds in Lemma G.1 is sharp at both $t = 0$ and $t \to \infty$.

Proof. Let $t > 0$. Let $\varphi(t)$ and $\Phi(t)$ respectively be the density and cumulative distribution function of $Z$. With $u = tx + x^2/2$ and $du = (t + x)dx$,
\[
\Phi(-t)/\varphi(t) = \int_0^\infty e^{-tx-x^2/2} dx = \int_0^\infty e^{-u} du = \int_0^\infty f_t(u^{-1/2})e^{-u} du,
\]
where $f_t(x) = (t^2 + 2/x^2)^{-1/2} = x(t^2x^2 + 2)^{-1/2}$ is a concave function of $x$. Thus,
\[
\Phi(-t)/\varphi(t) \leq f_t(\Gamma(1/2)) = f_t(\sqrt{\pi}) = (t^2 + 2/\pi)^{-1/2}.
\]

This gives the tail probability bound. From the well known $t(1 + t^2)^{-1} \varphi(t) \leq \Phi(-t)$, we also have
\[
\E[|Z - t|_+] = 2\{\varphi(t) - t\Phi(-t)\} \leq 2\varphi(t)/(1 + t^2).
\]

Define $J_k(t) = \int_0^\infty x^k e^{-x-x^2/(2t^2)} dx$. For the second tail moment, we have
\[
\E[|Z - t|^2] = 2\varphi(t) J_2(t)/t^3 = 2\Phi(-t) J_2(t)/(t^2 J_0(t)).
\]

As in Proposition 10 (i) in [SZ13] and its proof, (H.1) follows from $J_2(t)/J_0(t) \leq (1/2 + 1/t^2)$ due to the recursion $J_{k+1}(t) + t^{-2} J_{k+2}(t) = (k + 1) J_k(t)$ for $k \geq 0$.

H. Upper bound on the sparsity of the Lasso under the SRC

Proof of Proposition 3.12. The SRC (3.41) can be written as
\[
\max_{B \subset [p]: |B|, |S| \leq m} \phi_{\cond}(X_B^\top X_B - 1)(|S| + \epsilon_2 k) + \epsilon_1 k \leq 2(1 - \eta)^2 m.
\]

Let $g = (n\lambda)^{-1} X^\top P_B^\perp \varepsilon$ with elements $g_j \sim N(0, \sigma^2)$ satisfying $1/\sigma_j \geq t_\tau = \eta^{-1}\sqrt{(1 + \tau)2 \log(p/k)}$. Let $C_0 = \max_{B: |B|, |S| \leq m} \phi_{\cond}(X_B^\top X_B - 1)$ and
\[
\Omega = \{(4(1 - \eta))(|g| - \eta)_+ 1 + C_0 \| |g| - 1 + \|_2 < \epsilon_1 k + C_0 \epsilon_2 k\}.
\]

It follows from Lemma H.1 below that $|\hat{S} - S| < m$ in this event $\Omega$. Applying Lemma G.1, we find that
\[
4(1 - \eta)\E[\| |g| - \eta\|_1] \leq \frac{8(1 - \eta) p e^{-\eta^2 t_\tau^2/2}}{\sqrt{2\pi} t_\tau (1 + (\eta t_\tau)^2)} \leq \frac{\epsilon_1 k (k/p)^\tau}{1 + (\eta t_\tau)^2}
\]
with $\epsilon_1 = 8(1 - \eta)/\sqrt{2\pi} t_\tau$ and
\[
\E[\| |g| - 1\|_2^2] \leq \frac{4 e^{-t_\tau^2/2}}{t_\tau^2 (t_\tau^2 + 2) (2\pi t_\tau^2 + 4)^{1/2}} \leq \frac{\epsilon_2 k (k/p)^\tau}{1 + (\eta t_\tau)^2}
\]
with $\epsilon_2 = 4/(t_\tau^2 (2\pi t_\tau^2 + 4)^{1/2})$. Thus, $\P(\Omega)$ is no smaller than $1 - (k/p)^\tau/(1 + (\eta t_\tau)^2)$. Finally $\E[|\hat{S}|]$ is bounded from above by $|S| + m + \E[I_{\Omega^c} |\hat{S}|]$ so that combining $\E[I_{\Omega^c} |\hat{S}|] \leq p \P(\Omega^c)$ with the previous bound on $\P(\Omega^c)$ gives the upper bound on $\E[|\hat{S}|]$. 

\qed
The following lemma is a slight modification of [BZ18, Proposition 7.4].

**Lemma H.1** (Deterministic lemma). Let \( \lambda, \epsilon_1, \epsilon_2 > 0 \) and \( \eta \in (0, 1) \). Let \( \hat{\beta} \) be the Lasso \((3.34)\) with \( y = X\beta + \varepsilon \) and \( S = \text{supp}(\beta) \). If for \( g = X^T P_{\hat{S}} \varepsilon / (n\lambda) \) and \( C_0 = \max_{B : |B| \leq m} \phi_{\text{cond}}(X^T_B X_B) - 1 \) we have

\[
4(1 - \eta)\|((g - \eta)_+)\|_1 + C_0\|((g - 1)_+)\|_2^2 < \epsilon_1 k + C_0 \epsilon_2 k
\]

and the SRC \((3.41)\) holds, then \( |\hat{S} \setminus S| < m \).

**Proof.** The SRC \((3.41)\) can be written as \((H.1)\). Let \( \tilde{\beta} \) the oracle LSE satisfying \( \text{supp}(\beta) \subseteq S \) and \( X\tilde{\beta} = P_S y \). Let \( B \) satisfy

\[
S \cup \hat{S} \subseteq B \subseteq S \cup \{ j : |x_j^T (y - X\hat{\beta})/n| = \lambda \}.
\]

Let \( \Sigma = X^T X/n, B_1 = B \setminus S, u = (\beta - \tilde{\beta})/\lambda \) and \( v = \Sigma u \). By algebra,

\[
v_B^T \Sigma_{B,B}^{-1} v_B + v_{B_1}^T (\Sigma_{B,B}^{-1})_{B_1,B_1} v_{B_1} = v_S^T (\Sigma_{B,B}^{-1})_{S,S} v_S + 2u_{B_1}^T v_{B_1}.
\]

Let \( s = X^T (y - X\tilde{\beta})/(n\lambda) = g - v \). By the KKT conditions, \( s_j = \text{sgn}(u_j) \) for \( j \in B_1 \), so that \( u_{B_1} v_{B_1} = \sum_{j \in B_1} |u_j| |s_j g_j - 1| \leq v_B^T \Sigma_{B,B}^{-1} w_B \), where \( w \) is the vector with elements \( w_j = I_{\{ j \in B_1 \}} s_j (s_j g_j - 1)_+ \). By algebra,

\[
(v - w)^T \Sigma_{B,B}^{-1} (v - w)_B + v_{B_1}^T (\Sigma_{B,B}^{-1})_{B_1,B_1} v_{B_1}
\]

\[
\leq v_S^T (\Sigma_{B,B}^{-1})_{S,S} v_S + w_B^T \Sigma_{B,B}^{-1} w_B.
\]

It follows that

\[
\|v_S\|_2^2 + \|v_{B_1} - w_{B_1}\|_2^2 + \|w_{B_1}\|_2^2 \leq \phi_{\text{cond}}(\Sigma_{B,B})(\|v_S\|_2^2 + \|w_{B_1}\|_2^2).
\]

Moreover, as \( v_j - w_j = -s_j (s_j g_j - 1)_- \) for \( j \in B_1 \), \( \|v_{B_1}\|_2^2 = \|v_{B_1} - w_{B_1}\|_2^2 + \|w_{B_1}\|_2^2 \). This and the inequality above imply

\[
2\|v_{B_1} - w_{B_1}\|_2^2 \leq \phi_{\text{cond}}(\Sigma_{B,B} - I)(\|v_S\|_2^2 + \|w_{B_1}\|_2^2)
\]

As \( v = g - s \) and \( g_S = 0 \), \( \|v_S\|_2^2 = |S| \). We also have \( \|w_{B_1}\|_2^2 \leq \sum_{j=1}^p (s_j g_j - 1)_+^2 \) so that \( 2\|v_{B_1} - w_{B_1}\|_2^2 \leq C_0 (|S| + \|((g - 1)_+)\|_2^2) \). As \( s_j = \text{sgn}(u_j) \) and \( |v_j - w_j| = (1 - s_j g_j)_+ \) in \( B_1 \),

\[
2(1 - \eta)^2 |B_1| \leq 2\|v_{B_1} - w_{B_1}\|_2^2 + 4(1 - \eta) \sum_{j=1}^p (s_j g_j - \eta)_+ \leq C_0 (|S| + \|((g - 1)_+)\|_2^2) + 4(1 - \eta)\|((g - \eta)_+)\|_1 + \epsilon_1 k.
\]

Thus, by \((H.1)\), \( |B_1| \leq m \) implies \( |B_1| < m \). As \( |B_1| \) is allowed to change one-at-a-time along the Lasso path from \( \lambda = \infty \) and the condition on \( g \) is monotone in \( \lambda \), \( |B_1| < m \) holds for all penalty levels satisfying the condition on \( g \). For details of this argument see [Zha10, Proof of Lemma 1]. \( \square \)
I. Upper bound on the sparsity of the Lasso under the RE condition

Proof of Theorem 3.13. Let \( \mu = (1 + \tau)\sigma \sqrt{2 \log(ep/(s_0 \lor 1))}/n \) and \( \lambda = (1 + \gamma)\mu \). For each \( j \in [p] \) set \( g_j = (\tau + 1)\varepsilon^\top X e_j/n \). By the KKT conditions of the Lasso we have

\[
(\tau \varepsilon^\top X h + \|X h\|^2)/n \leq g^\top h - \lambda \|h_{S^c}\|_1 - \lambda \text{sgn}(\beta_{S^c})^\top h_S,
\]

where \( h = \hat{\beta}(\lambda) - \beta \). Define \( T = \{ u \in \mathbb{R}^p : \|u_{S^c}\|_1 < c_0 \sqrt{s_0} \lor 1 \|u\| \} \) as well as

\[
f_{\lambda,\mu}(\varepsilon) = \sup_{u \in T} \left( g^\top u - \mu \|u_{S^c}\|_1 - \lambda \text{sgn}(\beta_{S^c})^\top u_S \right) +,
\]

\[
g_{\lambda,\mu}(\varepsilon) = \sup_{u \notin T, \|X u\| > 0} \left( g^\top u - \mu \|u_{S^c}\|_1 - \lambda \text{sgn}(\beta_{S^c})^\top u_S - \gamma c_0 \sqrt{s_0} \lor 1 \|u\| \right) +
\]

where \( a_+ = \max(a, 0) \) for any real \( a \). Let \( \Omega \) be the event \( \Omega = \{ h \in T \} \) and \( I_\Omega \) be its indicator function. Using the elementary inequality \( 2ab - b^2 \leq a^2 \) we get

\[
(2\tau \varepsilon^\top X h + \|X h\|^2)/n \leq I_\Omega f_{\lambda,\mu}(\varepsilon)^2 / \text{RE}(S, c_0)^2 + I_\Omega g_{\lambda,\mu}(\varepsilon)^2.
\]

We now bound the expectation \( \mathbb{E}[f_{\lambda,\mu}(\varepsilon)^2] \). By simple algebra on each coordinate and the Cauchy-Schwarz inequality,

\[
f_{\lambda,\mu}(\varepsilon)^2 = \sum_{j \in S} (g_j - \lambda \text{sgn}(\beta_j))^2 + \sum_{j \notin S} (|g_j| - \mu)^2.
\]

Each \( g_j \) is centered, normal with variance at most \( \omega^2 = (1 + \tau)^2 \sigma^2/n \), hence Lemma G.1 implies that \( \mathbb{E}[f_{\lambda,\mu}(\varepsilon)^2] \leq s_0 (\lambda^2 + \omega^2) + (s_0 \lor 1) \omega^2 \), which is then bounded by \( 2^{-1}(\gamma c_0)^2 (s_0 \lor 1) \lambda^2 \) by the condition on \( c_0 \).

Note that by construction, the function \( \varepsilon \to g_{\lambda,\mu}(\varepsilon) \) is \( ((1+\tau)/\sqrt{n})\)-Lipschitz, so that by the Gaussian concentration inequality (see, e.g., [BLM13, Theorem 10.17]),

\[
\mathbb{E}[g_{\lambda,\mu}(\varepsilon)^2] = \int_0^{+\infty} \mathbb{P}\left[ g_{\lambda,\mu}(\varepsilon) > \sqrt{t} \right] dt \leq \int_0^{+\infty} \mathbb{P}\left[ \omega N(0, 1) > \sqrt{t} \right] dt = \omega^2/2,
\]

provided that the median of \( g_{\lambda,\mu}(\varepsilon) \) is zero. We now prove that the median is indeed zero. The event \( \{ f_{\lambda,\mu}(\varepsilon)^2 \leq 2\mathbb{E}[f_{\lambda,\mu}(\varepsilon)^2] \} \) has probability at least \( 1/2 \) thanks to Markov’s inequality. Furthermore, we proved above that \( 2\mathbb{E}[f_{\lambda,\mu}(\varepsilon)^2] \leq (c_0 \gamma)^2 (s_0 \lor 1) \lambda^2 \). On this event of probability at least \( 1/2 \), for any \( u \in T \) we have

\[
(g^\top u - \mu \|u_{S^c}\|_1 - \lambda \text{sgn}(\beta_{S^c})^\top u_S - (c_0 \gamma) \lambda \sqrt{s_0} \lor 1 \|u\|)_+ = 0.
\]

We have established that the median of \( g_{\lambda,\mu} \) is non-positive and the proof is complete. \( \square \)
J. Consistency of SURE for SURE in the Lasso case

Proof of Proposition 3.14. (i)-(iv) follow directly from Theorem 3.2. For (v), Markov’s inequality with the bound in (iii) followed by the bound \( \sigma^4 n \leq \mathbb{E}[\hat{R}_{\text{sure}}] \)
from (ii) implies

\[
|\hat{R}_{\text{sure}} - \mathbb{E}[\hat{R}_{\text{sure}}]|^2 \leq 4(n\alpha)^{-1}\sigma^4 n\mathbb{E}[\hat{R}_{\text{sure}}] \leq 4(n\alpha)^{-1}\mathbb{E}[\hat{R}_{\text{sure}}]^2
\]

with probability at least \( 1 - \alpha \), and \( \mathbb{E}[\hat{R}_{\text{sure}}] \leq (1 - 4(n\alpha)^{-1/2})^{-1}\hat{R}_{\text{sure}} \) on this event by the triangle inequality. The proof is completed using \( \mathbb{P}(|\hat{\text{SURE}} - \|X\hat{\beta}_{\lambda}^{(\lambda)} - \mu\|^2| \leq \gamma^{-1}\mathbb{E}[\hat{R}_{\text{sure}}]) \geq 1 - \gamma \). which follows by another application of Markov’s inequality.

□

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Fig 1: Approximate $\hat{\text{df}}$ for SVT, computed over 50 realisations of $(Z_1, \ldots, Z_m)$ for various values of $m$. The rightmost column is the exact formula from [CSLT13]. The value of $Y$ is the same over all 50 realisations.
Fig 2: Approximate $\text{div}(\hat{X}\hat{\beta})$ for the Elastic-net, computed over 50 realisations of $(z_1, \ldots, z_m)$ for various values of $m$. The rightmost column is the exact formula from [CSLT13]. Corresponding boxplots are visible in Figure 1. The value of $(X, y)$ is the same over all 50 realisations.