OUT-OF-SAMPLE ERROR ESTIMATION FOR M-ESTIMATORS WITH
CONVEX PENALTY

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Abstract. A generic out-of-sample error estimate is proposed for M-estimators regularized with
a convex penalty in high-dimensional linear regression where \((X, y)\) is observed and the dimension
\(p\) and sample size \(n\) are of the same order. The out-of-sample error estimate enjoys a relative
error of order \(n^{-1/2}\) in a linear model with Gaussian covariates and independent noise, either
non-asymptotically when \(p/n \leq \gamma\) or asymptotically in the high-dimensional asymptotic regime
\(p/n \to \gamma' \in (0, \infty)\). General differentiable loss functions \(\rho\) are allowed provided that the derivative
of the loss is 1-Lipschitz; this includes the least-squares loss as well as robust losses such as the
Huber loss and its smoothed versions. The validity of the out-of-sample error estimate holds either
under a strong convexity assumption, or for the L1-penalized Huber M-estimator and the Lasso
under a sparsity assumption and a bound on the number of contaminated observations.

For the square loss and in the absence of corruption in the response, the results additionally yield
\(n^{-1/2}\)-consistent estimates of the noise variance and of the generalization error. This generalizes,
to arbitrary convex penalty and arbitrary covariance, estimates that were previously known for the
Lasso.

Keywords: M-estimators, out-of-sample error estimation, parameter tuning, regularization, Huber
loss, robustness.

1. Introduction

Consider a linear model
\[
y = X \beta + \varepsilon
\]
where \(X \in \mathbb{R}^{n \times p}\) has iid \(N(0, \Sigma)\) rows and \(\varepsilon \in \mathbb{R}^n\) is a noise vector independent of \(X\). The entries
of \(\varepsilon\) may be heavy-tailed, for instance with infinite second moment, or follow Huber’s contamination
model with \(\varepsilon_i\) iid with cumulative distribution function (cdf) \(F(u) = (1 - q)P(N(0, \sigma^2) \leq u) + qG(u)\)
where \(q \in [0, 1]\) is the proportion of corrupted entries and \(G\) is an arbitrary cdf chosen by an
adversary. Since the seminal work of Huber in [29], a popular means to handle heavily-tails or
corruption of certain entries of \(\varepsilon\) is based on robust loss functions \(\rho : \mathbb{R} \to [0, +\infty)\) to construct M-
estimators \(\hat{\beta}\) by minimization of optimization problems of the form \(\hat{\beta} \in \arg \min_{b \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^n \rho(y_i - x_i^\top b)\) where \((x_i)_{i=1,...,n}\) are the rows of \(X\). Robustness against corruption of the above estimator
typically requires the convex loss \(\rho\) to grow linearly at \(\pm \infty\) and a well-studied example is the Huber
loss \(\rho_H(u) = \int_0^{|u|} \min(t, 1)dt\).

As we are interested in the high-dimensional regime where \(p\) is potentially larger than \(n\), we
also allow for convex penalty functions to leverage structure in the signal \(\beta\) and fight the curse of
dimensionality. The central object of the present paper is thus a penalized robust M-estimator of
the form
\[
\hat{\beta}(y, X) = \arg \min_{b \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^n \rho(y_i - x_i^\top b) + g(b) \right\}
\]
where \(\rho : \mathbb{R} \to \mathbb{R}\) is a convex differentiable loss function, and \(g : \mathbb{R}^p \to \mathbb{R}\) is a convex penalty. We
may write simply \(\hat{\beta}\) for \(\hat{\beta}(y, X)\) if the context is clear.

The main contribution of the present paper is the introduction of a generic out-of-sample error
estimate for penalized M-estimators of the form (1.2). Here, the out-of-sample error refers to the
random quantity

\[ \|\Sigma^{\frac{1}{2}}(\hat{\beta} - \beta)\|^2 = \mathbb{E}[(\hat{\beta} - \beta)^\top x_{\text{new}})^2 \mid (X, y)] \]

where \( x_{\text{new}} \) is independent of the data \((X, y)\) with the same distribution as any row of \( X \). Our goal is to develop such out-of-sample error estimate for \( \hat{\beta} \) in (1.2) with little or no assumption on the robust loss \( \rho \) and the convex penalty \( g \), in order to allow broad choices by practitioners for \((\rho, g)\).

We consider the high-dimensional regime where \( p \) and \( n \) are of the same order. The results of the present paper are non-asymptotic and assume that \( p/n \leq \gamma \in (0, \infty) \) for some fixed constant \( \gamma \) independent of \( n, p \). Although non-asymptotic, these results are applicable in the regime where \( n \) and \( p \) diverge such that

\[ \frac{p}{n} \to \gamma', \]

simply by considering a constant \( \gamma \geq \gamma' \). The analysis of the performance of convex estimators in the asymptotic regime (1.4) has received considerable attention in the last few years in the statistics, machine learning, electrical engineering and statistical physics communities. Most results available in the \( p/n \to \gamma' \) literature regarding \( M \)-estimators are either based on Approximate Message Passing (AMP) [1, 21, 11, 48, 12, 27] following the pioneering work [22] in compressed sensing problems, on leave-one-out methods [26, 3, 30, 25], or on the Gordon’s Gaussian min-max theorem (GMT) [42, 43, 44, 37]. The goal of these techniques is to summarize the performance and behavior of the \( M \)-estimator \( \hat{\beta} \) by a system of nonlinear equations with up to six unknown scalars (e.g., the system of [26] with unknowns \((r, c)\) for unregularized robust \( M \)-estimators, the system with unknowns \((\tau, \beta)\) of [37, Proposition 3.1] for the Lasso which dates back to [1], the system with unknowns \((\tau, \lambda)\) of [12, Section 4] for permutation-invariant penalties, or recently the system with six unknowns \((\alpha, \sigma, \gamma, \theta, \tau, r)\) of [40] in regularized logistic regression). Solving these nonlinear equations provide information about the risk \( \|\hat{\beta} - \beta\| \), and in certain cases asymptotic normality results for the coefficients of \( \hat{\beta} \) after a bias correction, see [12, e.g., Proposition B.3(iii)]. These systems of nonlinear equations depend the true coefficient vector \( \beta \) and the knowledge of \( \beta \) or its limiting empirical distribution is required to compute the solutions. For Ridge regression, results can be obtained using random matrix theory tools such as the Stieljes transform and limiting spectral distributions of certain random matrices [19, 20]. Our results are of a different nature, as they do not involve solving systems of nonlinear equations or their solutions. Instead, our results relate fully data-driven quantities to the out-of-sample error (1.3).

Additionally, most of the aforementioned works require isotropic design \((\Sigma = I_p)\), although there are notable exceptions for specific examples: isotropy can be relaxed for Ridge regularization [20], in unregularized logistic regression [51] and for the Lasso in sparse linear regression [13]. The techniques developed in the present paper do not rely on isotropy: general \( \Sigma \neq I_p \) is allowed without additional complexity.

We assume throughout the paper that \( \rho \) is differentiable and denote by \( \psi : \mathbb{R} \to \mathbb{R} \) the derivative of \( \rho \). We also assume that \( \psi \) is absolutely continuous and denote by \( \psi' \) its derivative. The functions \( \psi, \psi' \) act componentwise when applied to vectors, for instance \( \psi(y - X \bar{\beta}) = (\psi(y_i - x_i \top \bar{\beta}))_{i=1,\ldots,n} \). Throughout, \( \| \cdot \| \) is the Euclidean norm.

Contributions. The paper introduces a novel data-driven estimate of the out-of-sample error (1.3). The estimate depends on the data only through \( \hat{\psi} \triangleq \psi(y - X \bar{\beta}) \), the vector \( \Sigma^{-\frac{1}{2}}X \top \hat{\psi} \) and the derivatives of \( y \mapsto \beta \) and \( y \mapsto \psi(y - X \bar{\beta}) \) for fixed \( X \). For certain choices of \((\rho, g)\) these derivatives have closed forms, for instance in the case of the \( \ell_1 \)-penalized Huber \( M \)-estimator when \( \rho \) is the Huber loss, the estimator \( \hat{R} \) of the out-of-sample error (1.3) is

\[ \hat{R} = (|\hat{I}| - |\hat{S}|)^{-2}\left\{ \|\psi(y - X \bar{\beta})\|^2(2|\hat{S}| - p) + \|\Sigma^{-\frac{1}{2}}X \top \psi(y - X \bar{\beta})\|^2 \right\} \]
where \( \hat{S} = \{j \in [p] : \hat{\beta}_j \neq 0\} \) is the active set and \( \hat{I} = \{i \in [n] : \psi'(y_i - x_i^T \hat{\beta}) > 0\} \) is the set of inliers. Explicit formulae are also available for the Elastic-Net penalty \( g(b) = \lambda \|b\|_1 + \mu \|b\|_2 \) for any loss \( \rho \). For general choices of \((\rho, g)\), the derivatives can be approximated by a Monte Carlo scheme (cf. Section 2.11).

The estimate is valid under mild assumptions, namely: \( \psi \) is 1-Lipschitz, \( p/n \leq \gamma \) for some constant \( \gamma \) independent of \( n, p \) and that either (i) the penalty function \( g \) is \( \mu \)-strongly convex, (ii) the loss \( \rho \) is strongly convex and \( \gamma < 1 \), (iii.a) \( \hat{\beta} \) is the Lasso with square loss with a sparse \( \beta \), or (iii.b) \( \hat{\beta} \) is the \( \ell_1 \) penalized Huber \( M \)-estimator together with an additional assumption on the fraction of corrupted observations and sparsity of \( \beta \).

The proof arguments for the main theorem in Section 2 below provide new avenues to study \( M \)-estimators in the regime \( p/n \to \gamma' \). The results rely on novel moment inequalities (cf. Corollary 2.5 below) that let us directly bound the difference between quantities of interest (e.g., the out-of-sample error) and their estimates. These new techniques do not overlap with arguments typically used to analyse \( M \)-estimators when \( p/n \to \gamma' \) such as Approximate Message Passing (AMP) [1, 21, 11, 48, 12, 27], or the Gordon’s Gaussian Min-Max Theorem (GMT) [42, 43, 44, 37].

In the special case of the square loss, our estimate of the out-of-sample error coincides with previous estimates for the Ordinary Least-Squares [33], for the Lasso [1, 2, 37] and for \( \hat{\beta} = 0 \) [18]. Our results can be seen as a broad generalization of these estimates to (a) arbitrary covariance, (b) general loss function, including robust losses, and (c) general convex penalty. For the square loss, our results also yield generic estimates for the noise level and the generalization error \( E[(x_{new}^T \hat{\beta} - y_{new})^2|(X, y)] \). Most comparable to our results are the estimates of out-of-sample errors and other out-of-sample metrics studied in [38, 39, 49]. However, the accuracy of the estimates in these works is only guaranteed for smooth penalty functions [38, Theorem 3, Assumption 6], which excludes the \( \ell_1 \)-penalty, the Elastic-Net and the nuclear norm as regularizers.

Organization. Section 2 is devoted to the out-of-sample estimate \( \hat{R} \), the proof of its consistency, and explicit formulae for specific loss and penalty function commonly used in high-dimensional and robust statistics. Section 3 is devoted to the square loss for which additional results are available regarding estimation of the noise level and the generalization error. Sections 4 and 5 derive several Lipschitz properties to ensure existence of the derivatives as well as useful gradient identities for \( M \)-estimators. Sections 6 and 7 provide the main probabilistic results used in the paper.

Notation. The abbreviation a.s. means almost surely. Let \( I_d \) be the identity matrix of size \( d \times d \). For any \( p \geq 1 \), let \([p]\) be the set \([1, \ldots, p]\). Let \( \| \cdot \| \) be the Euclidean norm and \( \| \cdot \|_q \) the \( \ell_q \) norm of vectors. Let \( \| \cdot \|_{op} \) be the operator norm (largest singular value), \( \| \cdot \|_F \) the Frobenius norm. If \( M \) is positive semi-definite we also use the notation \( \phi_{\max}(M) \) and \( \phi_{\min}(M) \) for the largest and smallest eigenvalue. For any event \( \Omega \), denote by \( I(\Omega) \) its indicator function. For \( a \in \mathbb{R}, a_\pm = \max(0,a) \). Throughout the paper, we use \( C_1, C_2, \ldots \) to denote positive absolute constants, \( C_3(\gamma), C_4(\gamma), \ldots \) to denote constants that depend on \( \gamma \) only and for instance \( C_5(\gamma; \mu, \mu_g, \varphi, a_\pm) \) to denote a constant that depend on \( \{\gamma, \mu, \mu_g, \varphi, a_\pm\} \) only.

Canonical basis vectors are denoted by \( (e_i)_{i=1,..,n} \) or \( (e_l)_{l=1,..,n} \) for the canonical basis in \( \mathbb{R}^n \), and by \((e_j)_{j=1,..,p}\) or \((e_k)_{k=1,..,p}\) for the canonical basis vectors in \( \mathbb{R}^p \). Indices \( i \) and \( l \) are used to loop or sum over \([n] = \{1, \ldots, n\} \) only, while indices \( j \) and \( k \) are used to loop or sum over \([p] = \{1, \ldots, p\} \) only. This lets us use the notation \( e_i, e_l, e_j, e_k \) for canonical basis vectors in \( \mathbb{R}^n \) or \( \mathbb{R}^p \) as the index reveals without ambiguity whether the canonical basis vector lies in \( \mathbb{R}^n \) or \( \mathbb{R}^p \).

We will refer to Frechet differentiability for the usual notion of differentiability, i.e., \( f(x + h) = f(x) + \nabla f(x)^T h + o(\|h\|) \). This is stronger than, e.g., Gateaux differentiability for which linearity is not required.
2. Main result

Throughout, $\hat{\beta}$ is the estimator (1.2) with loss $\rho: \mathbb{R} \to \mathbb{R}$ and penalty $g: \mathbb{R}^p \to \mathbb{R}$. The goal of this section is to develop a generic estimator $\hat{R}$ for the Out-of-sample error $\|\Sigma^{1/2}(\hat{\beta} - \beta)\|^2$.

2.1. Assumptions.

**Assumption 2.1** (Loss function). The loss $\rho$ is convex and differentiable, and $\psi = \rho'$ is 1-Lipschitz with derivative denoted by $\psi'$ where the derivative exists.

This allows for a large class of non-robust and robust loss functions, including the square loss $\rho(u) = u^2/2$, the Huber loss $\rho_H(u) = \int_0^{|u|} \min(t,1)dt$ as well as smoothed versions of $\rho_H$. Since $\psi$ is 1-Lipschitz, $\psi'$ exist almost everywhere thanks to Rademacher’s theorem. Loss functions typically require a scaling parameter that depends on the noise level to obtain satisfactory risk bounds, see [16] and the references therein. For instance we consider in the main result below the loss

$$\rho(u) = \Lambda_*^2 \rho_H(\Lambda_*^{-1}u)$$

where $\rho_H$ is the Huber loss and $\Lambda_* > 0$ is a scaling parameter. Since for the Huber loss $\psi_H = \rho_H'$ is 1-Lipschitz, $\psi(u) = \rho(u) = \Lambda_* \psi_H(\Lambda_*^{-1}u)$ is also 1-Lipschitz. In short, scaling a given loss with a tuning parameter $\Lambda_*$ as in (2.1) does not change the Lipschitz constant of the first derivative of $\rho$, and the above assumption does not prevent using a scaling parameter $\Lambda_*$. Additionally, if the desired loss is such that $\psi$ is $L$-Lipschitz for some constant $L \neq 1$, one may replace $(\rho, g)$ by $(L^{-1}\rho, L^{-1}g)$ to obtain a 1-Lipschitz loss without changing the value of $\hat{\beta}$ in (1.2).

**Assumption 2.2** (Probability distribution). The rows of $X$ are iid $N(0, \Sigma)$ with $\Sigma$ invertible, $\varepsilon$ is independent of $X$, and $(X, y)$ has continuous distribution.

The Gaussian assumption is admittedly the strongest assumption required in this work. However arbitrary covariance $\Sigma$ is allowed, while a large body of related literature requires $\Sigma$ proportional to identity, see for instance [2, 11, 12, 40]. Allowing arbitrary $\Sigma$ together with general penalty functions is made possible by developing new techniques that are of a different nature than this previous literature; see the proof in Sections 2.8 and 2.9. We require that $(X, y)$ has continuous distribution in order to ensure that derivatives of certain Lipschitz functions of $(y, X)$ exist with probability one, again by Rademacher’s theorem. If $(X, y)$ does not have continuous distribution, one can always replace $y$ with $\tilde{y} = y + a\tilde{z}$ where $a$ is very small and $\tilde{z} \sim N(0, I_n)$ is sampled independently of $(\varepsilon, X)$. Hence the continuous distribution assumption is a mild technicality.

**Assumption 2.3** (Penalty). Assume either one of the following:

(i) $p/n \leq \gamma \in (0, +\infty)$ and the penalty $g$ is $\mu > 0$ strongly convex with respect to $\Sigma$, in the sense that any $b, b' \in \mathbb{R}^p, d \in \partial g(b)$ and $d' \in \partial g(b')$ satisfy $(d - d')^\top(b - b') \geq \mu \|\Sigma^{1/2}(b - b')\|^2$.

(ii) The penalty $g$ is only assumed convex, $p/n \leq \gamma < 1$ and $\mu > 0$ strongly convex in the sense that $(u - s)(\psi(u) - \psi(s)) \geq \mu_p(u - s)^2$ for all $u, s \in \mathbb{R}$.

(iii) For any constants $\varphi \geq 1, \gamma > 1, a_* > 0$ independent of $n, p$, assume $\text{diag}(\Sigma) = I_p, p/n \leq \gamma < (0, \infty)$ and $\phi_{\max}(\Sigma)/\phi_{\min}(\Sigma) \leq \varphi$. The penalty is $g(b) = n^{-1/2}\lambda\|b\|_1$ and either

(a) The loss is the squared loss $\rho(u) = u^2/2$, the noise is normal $\varepsilon \sim N(0, \sigma^2 I_n)$ and $\|eta\|_0 \leq s_* n$ where $s_* > 0$ is a small enough constant depending on $(\varphi, \gamma)$ only, and the tuning parameter $\lambda$ satisfies $\lambda \geq \sigma \lambda_*$ for some large enough constant $\lambda_* > 0$ depending only on $(\varphi, \gamma)$.

(b) The loss is $\rho(u) = \lambda_H^2 \rho_H(\lambda_H^{-1}u)$ for $\rho_H$ the Huber loss $\rho_H(u) = \int_0^{|u|} \min(t,1)dt$ and some tuning parameter $\lambda_H$. Furthermore $s_* > 0$ is a small enough constant depending on $(\varphi, \gamma, a_n)$ only such that there exists a set $O \subset [n]$ with $|O| + \|\beta\|_0 \leq s_* n$ such that the $n - |O|$ noise components $(\varepsilon_i)_{i \in [n] \setminus O}$ are iid $N(0, \sigma^2)$. The tuning parameters are
assumed to satisfy $\lambda/\lambda_H = a_*$ and $\lambda \geq \sigma \lambda_*$ for some large enough constant $\lambda_* > 0$
depending only on $(\varphi, \gamma, a_*)$.

Here and throughout the paper $\gamma, \mu, \mu_\varphi, a_\varphi \geq 0$ are constants independent of $n, p$.

Strong convexity on the penalty (i.e., (i) above) or strong convexity of the loss (i.e., (ii) above)
can be found in numerous other works on regularized $M$-estimators [21, 12, 50, among others].

In our setting, strong convexity simplifies the analysis as it grants existence of the derivatives of
$\hat{\beta}$ with respect to $(\mathbf{y}, \mathbf{X})$ "for free" thanks to the Lipschitz conditions obtained in Section 4.1.
Assumption (iii.a) above relaxes strong convexity on the penalty and (iii.b) relaxes strong convexity
on both the loss and penalty, by instead assuming a specific choice for $(\rho, g)$. Assumption (iii.a)
focuses on the Lasso under a sparsity assumption, while Assumption (iii.b) focuses the Huber loss and $\ell_1$
level together with an upper bound on the sparsity of $\beta$ and the number of corrupted
components of $\mathbf{e}$. In Assumption (iii.b), the uncorrupted observations are indexed in $[n] \setminus O$ and
the corrupted ones are those indexed in $O$. Assumption 2.3(iii.a) and (iii.b) provides non-trivial
examples for which our result holds without strong convexity on either the loss or the penalty.
Under Assumption 2.3(iii.b), the result holds provided that the corruption is not too strong and
the penalty $g$ (here the $\ell_1$ norm) is well suited to the structure of $\beta$ (here, the sparsity).

The generality in Assumption 2.3(i) and (ii) is obtained by leveraging the strong convexity
of either the loss or the penalty. Assumption 2.3(iii.a) and (iii.b) are more specific and show
that without strong convexity, our results still hold in these specific cases. The proof under
Assumption 2.3(iii.a) and (iii.b) leverages the special form of the loss and penalty and requires
a case-by-case analysis for these choices of $(\rho, g)$. Although we expect our main results to hold
without strong convexity for other penalty functions than the $\ell_1$ norm (e.g., the group Lasso norm
or indicator functions of convex sets by developing again case-by-case analysis), a global strategy
to characterize the pairs $(\rho, g)$ for which the results hold is currently out of reach.

2.2. Jacobians of $\hat{\psi}, \hat{\beta}$ at the observed data. Throughout the paper, we view the functions

$$
\hat{\beta} : \mathbb{R}^n \times \mathbb{R}^{n \times p} \to \mathbb{R}^p, \quad \hat{\psi} : \mathbb{R}^n \times \mathbb{R}^{n \times p} \to \mathbb{R}^n,
(\mathbf{y}, \mathbf{X}) \mapsto \hat{\beta}(\mathbf{y}, \mathbf{X}) \text{ in } (1.2),
(\mathbf{y}, \mathbf{X}) \mapsto \hat{\psi}(\mathbf{y}, \mathbf{X}) = \psi(\mathbf{y} - \mathbf{X}\hat{\beta}(\mathbf{y}, \mathbf{X}))
$$

as functions of $(\mathbf{y}, \mathbf{X})$, though we may drop the dependence in $(\mathbf{y}, \mathbf{X})$ and write simply $\hat{\beta}$ or
$\hat{\psi}$ if the context is clear. Here, recall that $\psi$ acts componentwise on the residuals $\mathbf{y} - \mathbf{X}\hat{\beta}$, so
that $\hat{\psi}(\mathbf{y} - \mathbf{X}\hat{\beta}) \in \mathbb{R}^n$ has components $\hat{\psi}(y_i - \mathbf{x}_i^\top \hat{\beta})_{i=1,...,n}$. The hat in the functions $\hat{\beta}$ and $\hat{\psi}$
above emphasize that they are data-driven quantities, and since they are functions of $(\mathbf{y}, \mathbf{X})$, the
directional derivatives of $\hat{\beta}$ and $\hat{\psi}$ at the observed data $(\mathbf{y}, \mathbf{X})$ are also observable quantities, for instance

$$
\frac{\partial}{\partial y_i} \hat{\beta}(\mathbf{y}, \mathbf{X}) = \left. \frac{d}{dt} \hat{\beta}(\mathbf{y} + t e_i, \mathbf{X}) \right|_{t=0}.
$$

Provided that they exist, the derivatives can be computed approximately by finite-difference or
other numerical methods; a Monte Carlo scheme to compute the required derivatives is given in
Section 2.11. We thus assume that the Jacobians

$$
V \overset{\text{def}}{=} \frac{\partial \hat{\psi}}{\partial \mathbf{y}}(\mathbf{y}, \mathbf{X}) = \left( \frac{\partial \hat{\psi}_l}{\partial y_i}(\mathbf{y}, \mathbf{X}) \right)_{(i,l) \in [n] \times [n]}, \quad \frac{\partial \hat{\beta}}{\partial \mathbf{y}}(\mathbf{y}, \mathbf{X}) = \left( \frac{\partial \hat{\beta}_l}{\partial y_i}(\mathbf{y}, \mathbf{X}) \right)_{(j,l) \in [p] \times [n]}
$$

are available. Above, $V$ is a matrix in $\mathbb{R}^{n \times n}$ with columns $\frac{\partial \hat{\psi}_l}{\partial y_i}(\mathbf{y}, \mathbf{X}), l = 1, ..., n$. Section 4.1
will make clear that the existence of such partial derivatives is granted, under our assumptions,
for almost every $(\mathbf{y}, \mathbf{X}) \in \mathbb{R}^n \times \mathbb{R}^{n \times p}$ by Rademacher’s theorem (cf. Proposition 4.2 below). For
brevity and if it is clear from context, we will drop the dependence in $(\mathbf{y}, \mathbf{X})$ from the notation, so
that the above Jacobians \( V = (\partial/\partial y)\hat{\psi} \in \mathbb{R}^{n \times m}, (\partial/\partial y)\hat{\beta} \in \mathbb{R}^{p \times n} \) as well as their entries \((\partial/\partial y_i)\hat{\psi}_i \) and \((\partial/\partial y_i)\hat{\beta}_j \) are implicitly taken at the currently observed data \((y, X)\). Next, define

\[
\hat{df} = \text{Tr}[(\partial/\partial y)X\hat{\beta}(y, X)],
\]

let \( \hat{I} = \{i \in [n] : \psi(y_i - x_i^\top \hat{\beta}) > 0\} \) be the set of detected inliers and \( \hat{O} = [n] \setminus \hat{I} \) the set of detected outliers. Finally, throughout the paper we denote by \( \psi' \in \mathbb{R}^n \) the vector with \( i \)-th component \( \psi(y_i - x_i^\top \hat{\beta}) \), \( \text{diag}(\psi') \in \mathbb{R}^{n \times n} \) the diagonal matrix with the entries of \( \psi' \) as diagonal entries, and \( h = \hat{\beta} - \beta \in \mathbb{R}^p \) the error vector so that the out-of-sample error that we wish to estimate is \( \|\Sigma^{1/2}h\|^2 \).

2.3. Main result. Equipped with the above notation for \( \hat{df} \) and the Jacobian \( V = (\partial/\partial y)\hat{\psi} \) at the observed data \((y, X)\), we are ready to state the main result of the paper.

**Theorem 2.1.** Let \( \hat{\beta} \) be the M-estimator (1.2). Define the estimate \( \hat{R} \) and the remainder \( \text{Rem} \) by

\[
\hat{R} \overset{\text{def}}{=} \text{Tr}[V]^{-2}\{\|\hat{\psi}\|^2(2\hat{df} - p) + \|\Sigma^{-\frac{1}{2}}X^\top \hat{\psi}\|^2\}, \quad \text{Rem} \overset{\text{def}}{=} \frac{\|\Sigma^{\frac{1}{2}}h\|^2 - \hat{R}}{\|\hat{\psi}\|^2/n + \|\Sigma^{\frac{1}{2}}h\|^2}.
\]

(i) If Assumptions 2.2, 2.1 and 2.3(i) hold then \( \mathbb{E}(|\frac{1}{n}\text{Tr}[V]|\text{Rem}| \leq C_6(\mu, \gamma)n^{-1/2} \).  
(ii) If Assumptions 2.2, 2.1 and 2.3(ii) hold, \( \mathbb{E}\{|\text{Rem}| \leq C_7(\mu, \gamma)n^{-1/2} \) and \( \frac{1}{n}\text{Tr}[V] \geq \mu_\rho(1 - \gamma) \) a.s. 
(iii) If Assumptions 2.2, 2.1 and 2.3(iii.a) or (iii.b) hold then \( \mathbb{E}\{|I\{\Omega\}\text{Rem}| \leq C_8(\varphi, \gamma, a_n)n^{-1/2} \) where \( I\{\Omega\} \) is the indicator of an event \( \Omega \) defined in the proof such that \( \mathbb{P}(\Omega) \to 1 \) as \( n, p \to +\infty \) while \( \{\varphi, \gamma, a_n\} \) remain fixed. Furthermore, \( \frac{1}{n}\text{Tr}[V] \geq 1 - d_\epsilon > 0 \) in \( \Omega \) for some constant \( d_\epsilon \) depending on \( \{\varphi, \gamma, a_n\} \) only.

The proof is given in Section 2.9. Recall that the target of estimation is the out-of-sample error \( \|\Sigma^{\frac{1}{2}}h\|^2 = \|\Sigma^{1/2} (\hat{\beta} - \beta)\|^2 \). In the regime of interest here with \( p/n \to \gamma' < 1 \), the risk \( \|\Sigma^{\frac{1}{2}}h\|^2 \) is typically of the order of a constant, see [26, 25, 21, 1, 44, 12] among others. When \( \|\hat{\psi}\|^2/n = \|\psi(y - X\hat{\beta})\|^2/n \) is also of order of a constant (e.g., with Huber loss \( \rho_H \) for which \( \sup_{t \in \mathbb{R}} |\psi(t)| = 1 \), Theorem 2.1 provides \( |\hat{R} - \|\Sigma^{1/2}h\|^2| = O_\varphi(n^{-\frac{1}{2}}) \) if the multiplicative factor \( \frac{1}{n}\text{Tr}[V] \) is bounded away from 0 in the sense that \( n/\text{Tr}[V] = O_\varphi(1) \). In particular, \( n/\text{Tr}[V] = O_\varphi(1) \) holds by Theorem 2.1 under Assumption 2.3(ii) and (iii).

The inequality in Theorem 2.1 is sharp for the Ordinary Least-Squares (OLS) with normal noise when \( p/n \leq \gamma < 1 \), i.e., for \( \rho(u) = u^2/2 \) and \( g(b) = 0 \). Assuming \( \varepsilon \sim N(0, \sigma^2 I_n) \), in this case we have

\[
\hat{df} = p, \quad \text{Tr}[(\partial/\partial y)\hat{\psi}/n] = n - p, \quad X^\top \hat{\psi} = 0, \quad \hat{R}/\sigma^2 = (n - p)^{-1}p\chi^2_{n-p},
\]

where \( \chi^2_{n-p} = \|\hat{\psi}\|^2/\sigma^2 = \|y - X\hat{\beta}\|^2/\sigma^2 \) has chi-square distribution with \( n - p \) degrees of freedom. Furthermore \( y - X\hat{\beta} \) is independent of \( \hat{\beta} \) and \( \hat{R}/\sigma^2 = (n - p)^{-1}p\chi^2_{n-p} \) has the same distribution as \( (n - p)^{-1}p\chi^2_{n-p} \), which is a chi-square distribution with \( n - p \) degrees of freedom. Since the standard deviation of \( \hat{R}/\sigma^2 \) equals \( (n - p)^{-1}p\sqrt{2(n - p)} \) and is equivalent to \( (1 - \gamma')^{-1}\gamma'\sqrt{2(1 - \gamma')}n^{-1/2} \) if \( p/n \to \gamma' < 1 \), this proves that \( \hat{R}/\|\Sigma^{1/2}h\|^2 \) incurs an unavoidable standard deviation of order \( \sigma^2 n^{-1/2} \). This result is valid for the OLS shows that an error term of order \( n^{-1/2} \) in the right hand side of Theorem 2.1 is unavoidable at least for this specific example. Theorem 2.1 is, in this sense, unimprovable.

The OLS is a simple example for which the inequality \( \hat{R} \approx \|\Sigma^{1/2}h\|^2 \) also follows, for instance, using the convergence of the spectral distribution of \( \Sigma^{-1/2}X^\top X\Sigma^{-1/2}/n \) to the Marchenko-Pastur law. Similarly, the approximation \( \hat{R} \approx \|\Sigma^{1/2}h\|^2 \) can be obtained for Ridge regression, that is, \( \rho(u) = u^2/2 \) and \( g(b) = \mu\|b\|^2 \), using again the limiting spectral distribution of \( \Sigma^{-1/2}X^\top X\Sigma^{-1/2}/n \). Outside of these cases, the approximation \( \hat{R} \approx \|\Sigma^{1/2}h\|^2 \) does not directly
Table 1. Explicit formulae for the factors $\hat{d}f$ and $\text{Tr}[(\partial/\partial y)\hat{\psi}]$ used in the out-of-sample estimate $\hat{R}$ for commonly used penalty functions. Here $\hat{I} = \{i \in [n] : \psi'(y_i - x_i^T\hat{\beta})\}$ is the set of inliers, $\hat{S} = \{j \in [p] : \hat{\beta}_j \neq 0\}$ is the set of active variables, $X_{\hat{S}}$ the submatrix of $X$ made of columns indexed in $\hat{S}$. See Propositions 2.3 and 2.4 for more details.

| Loss       | Penalty | $\hat{d}f$ | $\text{Tr}[(\partial/\partial y)\hat{\psi}]$ |
|------------|---------|------------|---------------------------------------------|
| $u^2/2$ (Square) | $\lambda\|b\|_1$ | $\|\hat{S}\|$ | $n - \|\hat{S}\|$ |
| $u^2/2$ (Square) | $\lambda\|b\|_1 + \mu\|b\|_2^2$ | $\text{Tr}[X_{\hat{S}}(X_{\hat{S}}^TX_{\hat{S}} + n\mu I)^{-1}X_{\hat{S}}^T]$ | $n - \|\hat{d}f\|$ |
| $\rho_H$ (Huber loss) | $\lambda\|b\|_1$ | $\|\hat{S}\|$ | $\|\hat{I}\| - \|\hat{S}\|$ |
| $\rho_H$ (Huber loss) | $\lambda\|b\|_1 + \mu\|b\|_2^2$ | $\text{Tr}[X_{\hat{S}}(X_{\hat{S}}^TDX_{\hat{S}} + n\mu I)^{-1}X_{\hat{S}}^TD]$ | $\|\hat{I}\| - \|\hat{d}f\|$ |
| Any | $\lambda\|b\|_1 + \mu\|b\|_2^2$ | $\text{Tr}[(2.9)]$ | $\text{Tr}[(2.10)]$ |

follow from the spectral distribution of $\Sigma^{-1/2}X^TX\Sigma^{-1/2}/n$. The present paper develops the theory to explain the approximation $\hat{R} \approx \|\Sigma^{1/2}h\|^2$ using simple first and second moment identities described in Section 2.8 which contains a proof sketch of Theorem 2.1.

2.4. On the range of the multiplicative factors in $\hat{R}$. Theorem 2.1 involves the multiplicative factors $\text{Tr}[(\partial/\partial y)\hat{\psi}]$ and $\hat{d}f$. The following result provides the possible range for these quantities.

**Proposition 2.2.** Assume that $\rho$ is convex differentiable and that $\psi = \rho'$ is 1-Lipschitz. For every fixed $X \in \mathbb{R}^{n \times p}$ the following holds.

- For almost every $y$, the map $y \mapsto \hat{\psi} = \psi(y - X\hat{\beta})$ is Frechet differentiable at $y$, and the Jacobian $V = (\partial/\partial y)\hat{\psi} \in \mathbb{R}^{n \times n}$ is symmetric psd with operator norm at most one so that $\text{Tr}[V] = \text{Tr}[(\partial/\partial y)\hat{\psi}] \in [0, n]$.
- If additionally Assumption 2.3(i) or (iii.b) holds then almost surely $\hat{d}f \leq |\hat{I}|$ where $\hat{I} = \{i \in [n] : \psi'(y_i - x_i^T\hat{\beta}) > 0\}$ is the set of inliers.

The proof of Proposition 2.2 is given in Section 9.1. For the square loss, $\hat{d}f$ is no more than the sample size $n$ since for any penalty, $\hat{d}f = \text{Tr}[(\partial/\partial y)X\hat{\beta}]$ is the divergence of a 1-Lipschitz function [5, e.g.]. The second point above states that this inequality is replaced by $\hat{d}f \leq |\hat{I}|$ for general loss functions, i.e., $n$ is replaced by the number of inliers.

2.5. $\hat{R}$ for certain examples of loss functions.

2.5.1. Square loss. As a first illustration of the above result, consider the square loss $\rho(u) = u^2/2$. As we will detail in Section 3 devoted to the square loss, $\hat{\psi} = y - X\hat{\beta}$ is the residuals and $V = (\partial/\partial y)\hat{\psi} = I_n - X(\partial/\partial y)\hat{\beta}$ by the chain rule so that $\hat{R}$ reduces to

$$\hat{R} = (n - \hat{d}f)^{-2}\{\|\hat{\psi}\|^2(2\hat{d}f - p) + \|\Sigma^{-\frac{1}{2}}X^T\hat{\psi}\|^2\}.$$ 

Above, $\hat{d}f = \text{Tr}[(\partial/\partial y)X\hat{\beta}]$ is the usual effective number of parameters or effective degrees-of-freedom of $\hat{\beta}$ that dates back to Stein [41]. This estimator of the out-of-sample error for the square loss was known only for two specific penalty functions $g$. The first is $g = 0$ [33] in which case $\hat{\beta}$ is the Ordinary Least-Squares and $\hat{d}f = p$. The second is $g(b) = \lambda\|b\|_1$ [2, 37], in which case $\hat{\beta}$ is the Lasso and $\hat{d}f = |\{j \in [p] : \hat{\beta}_j \neq 0\}|$. For $g$ not proportional to the $\ell_1$-norm, the above result is to our
knowledge novel, even restricted to the square loss. As we detail in Section 3, the algebraic nature of the square loss leads to additional results for noise level estimation and adaptive estimation of the generalization error. Here, adaptive means without knowledge of $\Sigma$. To our knowledge, the estimate $\hat{R}$ for general loss functions ($\rho$ different than the square loss) is new.

2.5.2. Huber loss. As a second illustration, consider the Huber loss $\rho_H(u) = \int_0^{|u|} \min(t, 1) dt$, i.e.,

$$\rho_H(u) = \frac{u^2}{2} \text{ for } |u| \leq 1 \quad \text{and} \quad \rho_H(u) = (|u| - 1/2) \text{ for } |u| > 1.$$  

(2.7)

By the chain rule in (2.21) below, using (2.19) and noting that $\text{diag}(\psi') = \text{diag}(\psi'^2)$ for the Huber loss, $\text{Tr}[V] = \text{Tr}[\partial(\partial/y)\psi] = \text{Tr}[\text{diag}(\psi')(I_n - (\partial/\partial y)X\beta)] = |\hat{I}| - \hat{d}f$ where $I = \{i \in [n] : \psi'(y_i - x_i^\top \beta) > 0\}$. The out-of-sample estimate $\hat{R}$ becomes

$$\hat{R} = (|\hat{I}| - \hat{d}f)^{-2}\{|\psi|^2(2\hat{d}f - p) + \|\Sigma^{-\frac{1}{2}}X^\top \psi\|^2\}.$$  

This conveniently mimics the estimate available for the square loss, with the sample size $n$ replaced by the number of inliers $|\hat{I}|$. If a scaled version of the Huber loss is used, i.e., with loss $\rho(y) = \Lambda^2 \rho_H(\Lambda^{-1}u)$ for some scaling parameter $\Lambda > 0$, then the previous display still holds.

2.6. When is $\text{Tr}[V] = \text{Tr}[\partial(\partial/y)\psi]/n$ too small or 0? We emphasize that the above result does not provide guarantees against all forms of corruption in the data, and $\hat{R}$ may produce incorrect inferences (or be undefined due to division by 0) if the multiplicative factor $(\frac{1}{n} \text{Tr}[V])^2 = (\frac{1}{n} \text{Tr}[\partial(\partial/y)\psi])^2$ is too small or equal to 0. This issue does not arise under Assumption 2.3(ii) or (iii), as in this case Theorem 2.1 grants $\frac{1}{n} \text{Tr}[V]$ larger than some positive constant with high probability.

Recall that $\frac{1}{n} \text{Tr}[V] = \frac{1}{n} \text{Tr}[\partial(\partial/y)\psi] \in [0, 1]$ by Proposition 2.2. To exhibit situations for which $\frac{1}{n} \text{Tr}[\partial(\partial/y)\psi]$ is close to 0 under Assumption 2.3(i), by the chain rule (2.21) below we have

$$\frac{1}{n} \text{Tr}[V] = \frac{1}{n} \text{Tr}[\partial(\partial/y)\psi] = \frac{1}{n} \text{Tr}[\text{diag}(\psi')(I_n - X(\partial/\partial y)\beta)].$$  

Hence the above multiplicative factor is equal to 0 when $\text{diag}(\psi') = 0$, i.e., $\psi'(y_i - x_i^\top \beta) = 0$ for all observations $i = 1, ..., n$: If all observations are classified as outliers by the minimization problem (1.2) then $\hat{R}$ is undefined and cannot be used. On the other hand, by Theorem 2.1 under Assumption 2.3(i) the relationship

$$\left(\frac{1}{n} \text{Tr}[\partial(\partial/y)\psi]\right)^2 \|\Sigma^{\frac{1}{2}}h\|^2 - \hat{R} \leq \text{Rem}(\|\Sigma^{\frac{1}{2}}h\|^2 + \|\tilde{\psi}\|^2/n)$$  

(2.8)

always holds with $\text{Rem} = O_p(n^{-1/2})$, which suggests that $(\frac{1}{n} \text{Tr}[V])^2 = (\frac{1}{n} \text{Tr}[\partial(\partial/y)\psi])^2$ must be bounded away from 0 in order to obtain meaningful upper bounds on $\|\Sigma^{\frac{1}{2}}h\|^2 - \hat{R}$. If the loss is strongly convex and $\gamma < 1$ as in Assumption 2.3(ii), or under Assumption 2.3(iii.a) or (iii.b) for $\ell_1$ penalty with square or Huber loss, the factor $(\frac{1}{n} \text{Tr}[\partial(\partial/y)\psi])^2$ is bounded away from 0 as noted in the second claim of Theorem 2.1. However, $(\frac{1}{n} \text{Tr}[\partial(\partial/y)\psi])^2$ is not necessarily bounded away from 0 under Assumption 2.3(i): Indeed it is easy to construct an example where $\psi'(y_i - x_i^\top \beta) = 0$ for all $i \in [n]$ with high probability, for instance for the Huber loss $\rho = \rho_H$ defined in (2.7) with penalty $g(b) = K\|b - \alpha\|^2$ for some large $K$ and some vector $\alpha \in \mathbb{R}^p$ with large distance $\|\alpha - \beta\|$ (this is a purposely poor choice of penalty function that will induce a large error $\|\Sigma^{\frac{1}{2}}h\|^2$). This example highlights that the above result does not provide estimation guarantees against all forms of corruption under Assumption 2.3(i) without further assumption: If the corruption is so strong that all observations are outliers and $\text{Tr}[\partial(\partial/y)\psi] = 0$ then $\hat{R}$ is undefined and the inequality of Theorem 2.1 is unusable to estimate or bound from above the out-of-sample error.
2.7. Closed form expression for specific choices of \((\rho, g)\). The multiplicative factors \(\text{Tr}[(\partial / \partial y) \hat{\psi}]\) and \(\text{df} = \text{Tr}[(\partial / \partial y) X \hat{\beta}]\) have explicit closed form expressions for particular choices of \((\rho, g)\). We now provide such examples; a summary is provided in Table 1. The next section provides a general method to approximate \(\text{Tr}[(\partial / \partial y) \hat{\psi}]\) and \(\text{df}\) for arbitrary \((\rho, g)\) when no closed form expressions are available.

**Proposition 2.3.** Assume that \(\psi\) is 1-Lipschitz and consider an Elastic-Net penalty of the form \(g(b) = \mu \|b\|^2 / 2 + \lambda \|b\|_1\) for \(\mu > 0, \lambda \geq 0\). For almost every \((y, X)\), the map \(y \mapsto X \hat{\beta}\) is differentiable at \(y\) and

\[
(\partial / \partial y) X \hat{\beta} = X_S (X_S^\top \text{diag} (\psi') X_S + n \mu I_{|S|} )^{-1} X_S^\top \text{diag} (\psi')
\]

where \(S = \{ j \in [p] : \hat{\beta}_j \neq 0 \}\) and \(X_S\) is the submatrix of \(X\) obtained made of columns indexed in \(S\), and

\[
\frac{\partial \hat{\psi}}{\partial y} = \text{diag}(\psi')^{\frac{1}{2}} [I_n - \text{diag}(\psi')^{\frac{1}{2}} X_S (X_S^\top \text{diag} (\psi') X_S + n \mu I_{|S|} )^{-1} X_S^\top \text{diag} (\psi')^{\frac{1}{2}} ] \text{diag} (\psi')^{\frac{1}{2}}.
\]

The proof is given in Section 9.2. For the Elastic-Net penalty, the factors \(\text{df} = \text{Tr}[(\partial / \partial y) X \hat{\beta}]\) and \(\text{Tr}[(\partial / \partial y) \hat{\psi}]\) appearing in the out-of-sample estimate \(\hat{R}\) have thus reasonably tractable forms and can be computed efficiently by inverting a matrix of size \(\hat{S}\) once the elastic-net estimate \(\hat{\beta}\) has been computed. The above estimates for general loss functions are closely related to the formula for \((\partial / \partial y) X \hat{\beta}\) known for the Elastic-Net with square loss \([46, \text{Equation (28)}] [6, \text{Section 3.5.3}], \) the only difference being several multiplications by the diagonal matrix \(\text{diag}(\psi')\). Closed form expressions can also be obtained for different penalty functions, such as the Group-Lasso penalty, by differentiating the KKT conditions as explained in [7] for the square loss.

For the Huber loss with \(\ell_1\)-penalty, these multiplicative factors are even simpler, as shown in the following proposition. We keep using the notation \(\hat{I} = \{ i \in [n] : \hat{\beta}_i > 0 \}\) for the set of inliers (the set of outliers being \([n] \setminus \hat{I}\) ), and \(\hat{S} = \{ j \in [p] : \hat{\beta}_j \neq 0 \}\) for the set of active covariates.

**Proposition 2.4.** Let \(\rho(u) = n \lambda^2 \rho_H (\sqrt{n} \lambda) u\) where \(\rho_H\) is the Huber loss and let \(g(b) = \lambda \|b\|_1\) be the penalty for \(\lambda, \lambda > 0\). For almost every \((y, X)\), the functions \(y \mapsto \hat{I}, y \mapsto \hat{S}\) and \(y \mapsto \text{diag}(\psi')\) are constant in a neighborhood of \(y\) and \(\hat{Q} = \text{diag}(\psi') (\partial / \partial y) X \hat{\beta}\) is the orthogonal projection onto the column span of \(\text{diag}(\psi') X_S\). Furthermore \((\partial / \partial y) \hat{\psi} = \text{diag}(\psi') - \hat{Q}\) and the multiplicative factors appearing in \(\hat{R}\) satisfy for almost every \((y, X)\)

\[
\text{df} = \text{Tr}[\text{diag}(\psi') (\partial / \partial y) X \hat{\beta}] = |\hat{S}|, \quad \text{Tr}[(\partial / \partial y) \hat{\psi}] = |\hat{I}| - |\hat{S}| \geq 0.
\]

The proof is given in Section 9.2. Proposition 2.4 implies that for the Huber loss with \(\ell_1\)-penalty, the out-of-sample error estimate \(\hat{R}\) becomes simply

\[
\hat{R} = (|\hat{I}| - |\hat{S}|)^{-2} \{ \|\psi\|^2 (2|\hat{S}| - p) + \|\Sigma^{-\frac{1}{2}} X^\top \hat{\psi}\|^2 \}.
\]

For the square-loss and identity covariance, the above estimate was known [2, 37] with \(|\hat{I}|\) replaced by \(n\) In hindsight the extension of this estimate to the Huber loss is natural: the sample size should be replaced by the number of observed inliers \(|\hat{I}|\).

2.8. **Proof ingredients and a new probabilistic inequality.** Preliminaries for the proofs are twofold. First several Lipschitz properties are derived, to make sure that the derivatives used in the proofs exist almost surely. This is done in Section 4.1. Second, without loss of generality we may assume that \(\Sigma = I_p\), replacing if necessary \((X, \beta, \hat{\beta}, g)\) by \((X^*, \beta^*, \hat{\beta}^*, g^*)\) as follows,

\[
X \sim X^* = X \Sigma^{-\frac{1}{2}}, \quad g(\cdot) \sim g^*(\cdot) = g(\Sigma^{-\frac{1}{2}}(\cdot)), \quad \beta \sim \beta^* = \Sigma^{\frac{1}{2}} \beta, \quad \beta \sim \beta^* = \Sigma^{\frac{1}{2}} \beta.
\]
This change of variable leaves the quantities \( \{y, df, \hat{\psi}, X\hat{\beta}, \|\Sigma^{-\frac{1}{2}} X^\top \hat{\psi}\|^2, \|\Sigma^{\frac{1}{2}} h\|^2, \text{Tr}[V]\} \) unchanged, so that Theorem 2.1 holds for general \( \Sigma \) if it holds for \( \Sigma = I_p \) after the change of variable in (2.12). Next, throughout the proof we consider the scaled version of \( \eta \) and the error vector \( h \) given by

\[
(2.13) \quad r = n^{-\frac{1}{2}} \hat{\psi} = n^{-\frac{1}{2}} \psi (y - X\hat{\beta}), \quad h = \hat{\beta} - \beta
\]

so that \( \|r\|^2 \) and \( \|h\|^2 \) are of the same order.

At this point the main ingredients of the proof are threefold. The first ingredient is the following.

**Proposition 6.5.** Let \( X = (x_{ij}) \in \mathbb{R}^{n \times p} \) with iid \( N(0,1) \) entries and \( \eta : \mathbb{R}^{n \times p} \to \mathbb{R}^p, \rho : \mathbb{R}^{n \times p} \to \mathbb{R}^n \) two vector valued functions, with weakly differentiable components \( \eta_1, \ldots, \eta_p \) and \( \rho_1, \ldots, \rho_n \). Then

\[
\mathbb{E} \left[ \left( \rho^\top X \eta - \sum_{i=1}^{n} \sum_{j=1}^{p} \frac{\partial (\rho_i \eta_j)}{\partial x_{ij}} \right)^2 \right] = \mathbb{E} \left[ \|\rho\|^2 \|\eta\|^2 + \sum_{i=1}^{p} \sum_{j=1}^{p} \sum_{k=1}^{n} \frac{\partial (\rho_i \eta_j)}{\partial x_{ik}} \frac{\partial (\rho_i \eta_k)}{\partial x_{ij}} \right]
\]

\[
(6.6) \leq \mathbb{E} \left[ \|\rho\|^2 \|\eta\|^2 + \sum_{j=1}^{p} \sum_{i=1}^{n} \left\| \frac{\partial (\rho^\top)}{\partial x_{ij}} \right\|_F^2 \right]
\]

provided that the second line is finite, where for brevity we write \( \rho = \rho(X), \eta = \eta(X) \), and similarly for the partial derivatives (i.e., omitting the dependence in \( X \)).

The proof is given in Section 6. In practice for the proofs of the main theorems, we take

\[
(2.14) \quad \eta(X) = (\|r\|^2 + \|h\|^2)^{-1/2} X^\top r \quad \text{and} \quad \rho(X) = (\|r\|^2 + \|h\|^2)^{-1/2} r
\]

with \( r, h \) defined in (2.13). The equality in (6.6) is a matrix generalization of [41, Eq. (8.6)], [6]. Its proof relies on Gaussian integrations by parts and presents no difficulty, although it requires some bookkeeping for the different summation signs and indices. The result of [6], that covers the case \( p = 1, \eta = 1 \), is recalled in Proposition 6.3. Although the above matrix formulation is new and particularly useful for our purpose, it is essentially equivalent to the for the partial derivatives (i.e., omitting the dependence in \( X \)).

The second ingredient is the following novel probabilistic inequality, which is the main probabilistic contribution of the present paper.

**Theorem 7.2.** Assume that \( X \) has iid \( N(0,1) \) entries, that \( \rho : \mathbb{R}^{n \times p} \to \mathbb{R}^n \) is weakly differentiable and that \( \|\rho\| \leq 1 \) almost everywhere. Then

\[
(7.4) \quad \mathbb{E} \|\rho\|^2 - \sum_{j=1}^{p} \left( \rho^\top X e_j - \sum_{i=1}^{n} \frac{\partial \rho_i}{\partial x_{ij}} \right)^2 \leq C_9 \mathbb{E} \left[ 1 + \sum_{i=1}^{n} \sum_{j=1}^{p} \| \frac{\partial \rho_i}{\partial x_{ij}} \|^2 \right]^{1/2} \sqrt{p} + C_{38} \sum_{i=1}^{n} \sum_{j=1}^{p} \| \frac{\partial \rho_i}{\partial x_{ij}} \|^2
\]

where \( C_{38} > 0 \) is an absolute constant.

The proof of Theorem 7.2 is given in Section 7. To our knowledge, inequality (7.4) is novel. In the simplest case, if \( \rho \) is constant with \( \|\rho\| = 1 \) then (7.4) reduces to \( \mathbb{E} [\chi_p^2 - p] \leq C_{10} \sqrt{p} \) and the dependence in \( \sqrt{p} \) is optimal, so that (7.4) is in a sense unimprovable. The flexibility of inequality (7.4) is that the left hand side of (7.4) is provably of order \( \sqrt{p} \), as in the case of \( \mathbb{E} [\chi_p^2 - p] \), as long as the derivatives of \( \rho \) do not vary too much in the sense that \( \mathbb{E} \sum_{i=1}^{n} \sum_{j=1}^{p} \| \frac{\partial \rho_i}{\partial x_{ij}} \|^2 \leq C_{11} \) for some constant independent of \( n, p \). This inequality holds for instance for all \( (C_{11}/n)^{1/2} \)-Lipschitz functions \( \rho : \mathbb{R}^{n \times p} \to \mathbb{R}^n \) since the squared Frobenius norm of the Jacobian of \( \rho \) is bounded by \( n \) times the square of the Lipschitz constant. A right-hand side of order \( \sqrt{p} \) in (7.4) would be expected if the \( p \) terms

\[
A_j = \|\rho\|^2 - (\rho^\top X e_j - \sum_{i=1}^{n} \frac{\partial \rho_i}{\partial x_{ij}})^2
\]
were mean-zero and independent, thanks to \(\mathbb{E}[(\sum_{j=1}^{p} A_j)^2] = \sum_{j=1}^{p} \mathbb{E}[A_j^2]\) by independence. The surprising feature of (7.4) is that such bound of order \(\sqrt{p}\) holds despite the intricate, nonlinear dependence between \(A_j\) and the \(p-1\) other terms \((A_k)_{k \neq j}\) through the \((C_{11}/n)^{1/2}\)-Lipschitz function \(\rho\) and its partial derivatives. We now state two useful inequalities that follow directly by combining Theorem 7.2 and Proposition 6.5 for \(\eta = X^\top \rho\).

**Corollary 2.5.** Assume that \(X\) has iid \(N(0,1)\) entries, that \(\rho : \mathbb{R}^{n \times p} \to \mathbb{R}^n\) is weakly differentiable and that \(\|\rho\| \leq 1\) almost everywhere. Then

\[
\mathbb{E}\left\|X^\top \rho - p\|\rho\|^2\right\| - 2 \sum_{j=1}^{p} \left(\sum_{i=1}^{n} \frac{\partial \rho_i}{\partial x_{ij}}\right)^2 - 2 \sum_{j=1}^{p} \sum_{i=1}^{n} \rho_i e_j^\top X^\top \frac{\partial \rho_j}{\partial x_{ij}} \leq C_{12} \text{RHS},
\]

\[
\left|\left|\sum_{j=1}^{p} \rho_j^\top X e_j \sum_{i=1}^{n} \frac{\partial \rho_i}{\partial x_{ij}} - \sum_{j=1}^{p} \left(\sum_{i=1}^{n} \frac{\partial \rho_i}{\partial x_{ij}}\right)^2 - \sum_{j=1}^{p} \sum_{i=1}^{n} \rho_i e_j^\top X^\top \frac{\partial \rho_j}{\partial x_{ij}}\right|\right| \leq C_{13} \text{RHS}
\]

where \(\text{RHS} = \mathbb{E}\left[\sum_{i=1}^{n} \left(\sum_{j=1}^{p} \frac{\partial \rho_i}{\partial x_{ij}}\right)^2\right] + \sqrt{p+n} + \mathbb{E}\left[\|p + \|X\|_2^2\right]_{\text{op}} \sum_{i=1}^{n} \sum_{j=1}^{p} \|\frac{\partial \rho_j}{\partial x_{ij}}\|^2_1/2.\]

The proof is given in Section 7. Inequalities (6.6), (7.4), (2.15) and (2.16) involve derivatives with respect to the entries of \(X\). It might thus be surprising at this point that Theorem 2.1 and the estimate \(\hat{R}\) in (2.5) involve the derivatives of \((\hat{\psi}, \hat{\beta})\) with respect to \(y\) only, and no derivatives with respect to the entries of \(X\). The third major ingredient of the proof is to provide gradient identities between the derivatives of \(\hat{\beta}, \hat{\psi}\) with respect to \(y\) and those with respect to \(X\), by identifying certain perturbations of the data \((y, X)\) that leave \(\hat{\beta}\) or \(\hat{\psi}\) unchanged. For instance, Corollary 5.1 shows that \(\hat{\psi}\) stays the same and \(\hat{\beta}\) is still solution of the optimization problem (1.2) if the observed data \((y, X)\) is replaced by \((y + \beta^\top v, X + ve_j^\top)\) for any canonical basis vector \(e_j \in \mathbb{R}^p\) and any direction \(v \in \mathbb{R}^n\) with \(v^\top \psi = 0\). If \(\hat{\psi}(y, X)\) and \(\hat{\beta}(y, X)\) are Frechet differentiable with respect to \((y, X)\), such perturbations that leaves \(\hat{\beta}, \hat{\psi}\) unchanged provide relationship between the partial derivatives with respect to \(y\) and the partial derivatives with respect to entries of \(X\). If \(\hat{\beta}^0 = \hat{\beta}(y^0, X^0)\), \(\hat{\psi}^0 = \hat{\psi}(y^0, X^0)\) and similiary for \(\psi^0\), another perturbation that leaves \(\hat{\beta}\) unchanged at \((y^0, X^0)\) is

\[
y(t) = y + t(U \text{diag}(\psi^0) X \beta - X^\top \psi^0), \quad X(t) = X + tU \text{diag}(\psi^0)
\]

as \(t \to 0\) for any fixed \(U \in \mathbb{R}^{n \times n}\), in the sense that \(\frac{d}{dt} \hat{\beta}(y(t), X(t))|_{t=0} = 0\) when \(\mu > 0\) (i.e., the penalty is strongly convex). A more convenient form of such results was developed in [4] after the first version of the present manuscript appeared; we include it in the next lemma for convenience as it makes the proofs easier to read.

**Lemma 2.6** (Variant of Theorem 1 in [4]). Let \(\mu \geq 0\) (allowing \(\mu = 0\)). Let \(\hat{\beta}\) be the M-estimator (1.2) with convex loss \(\rho\) and \(\mu\)-strongly convex penalty \(g\) with respect to a positive definite \(\Sigma\) in the sense of Assumption 2.3(i). Assume that \(\hat{\beta}(y, X)\) and \(\hat{\psi}(y, X)\) are Frechet differentiable at \((y^0, X^0)\). Let \(\hat{\beta}^0 = \hat{\beta}(y^0, X^0)\) and \(\psi^0 = \psi(y^0 - X^0 \beta^0)\), as well as the \(n \times n\) diagonal matrix \(D^0 = \text{diag}(\psi^0) = \text{diag}(\psi_3^0, ..., \psi_n^0)\) where \(\psi_i^0 = \psi^0(y^0_i - x_i^0 \beta^0)\) for each \(i = 1, ..., n\). If \(\psi\) is continuously differentiable and \(\mu n \Sigma + X^0 \text{diag}(\psi^0) X^0\) is positive definite then there exists a \(p \times p\) matrix \(\hat{A}(y^0, X^0)\) depending on \((y^0, X^0)\) such that

\[
\frac{\partial \beta_i}{\partial x_{ij}}(y^0, X^0) = \hat{A}(y^0, X^0) e_j \psi^0_i - X^0 D^0 e_j \beta^0
\]

for all \(i \in [n], j \in [p]\),

\[
\frac{\partial \psi_i}{\partial y_j}(y^0, X^0) = \hat{A}(y^0, X^0) [X^0^\top D^0 e_i]
\]

for all \(l \in [n]\),

\[
\|\Sigma^{1/2} \hat{A}(y^0, X^0) \Sigma^{1/2}\|_{\text{op}} \leq \phi_{\min}(\mu n I_p + \Sigma^{-1/2} X^0 D^0 X \Sigma^{-1/2})^{-1}.
\]

If \(\psi\) is only 1-Lipschitz (but not necessarily continuously or everywhere differentiable) and the function \((y, X) \mapsto \hat{\beta}(y, X)\) is Lipschitz in some open set \(U\), then for almost every \((y^0, X^0)\) in \(U\),

\[
\|\Sigma^{1/2} \hat{A}(y^0, X^0) \Sigma^{1/2}\|_{\text{op}} \leq \phi_{\min}(\mu n I_p + \Sigma^{-1/2} X^0 D^0 X \Sigma^{-1/2})^{-1}.
\]
the chain rule
\begin{equation}
\frac{\partial \hat{\psi}}{\partial x_{ij}}(y^0, X^0) = D^0[-X^0 \frac{\partial \beta}{\partial x_{ij}}(y^0, X^0) - e_{ij}\beta], \quad \frac{\partial \hat{\psi}}{\partial y_{ij}}(y^0, X^0) = D^0[e_{i} - X^0 \frac{\partial \beta}{\partial y_{ij}}(y^0, X^0)]
\end{equation}
and (2.18)-(2.19)-(2.20) still hold for some $\tilde{A}(y^0, X^0) \in \mathbb{R}^{p \times p}$ when the right-hand side of (2.20) is finite.

We provide a short proof in Section 5. We will omit the $0$ superscript and the explicit dependence on $(y, X)$ for brevity, and write simply using the chain rule
\begin{equation}
\frac{\partial \mathbf{a}}{\partial x_{ij}} = \hat{A}[e_j \hat{\psi}_i - X^\top \text{diag}(\psi')e_i \hat{\beta}_j], \quad \frac{\partial \mathbf{a}}{\partial y_{ij}} = \hat{A}X^\top \text{diag}(\psi')e_i,
\end{equation}
\begin{equation}
\frac{\partial \hat{\psi}}{\partial x_{ij}} = -\text{diag}(\psi')X\hat{A}e_j \hat{\psi}_i - Ve_i \hat{\beta}_j, \quad \frac{\partial \hat{\psi}}{\partial y_{ij}} = Ve_i \quad \text{where } V = \text{diag}(\psi') - \text{diag}(\psi')X\hat{A}X^\top \text{diag}(\psi').
\end{equation}

Since the matrix $\hat{A}$ is the same in the derivatives with respect to $X$ and with respect to $y$, (2.22) provides relationships between the partial derivatives with respect to $X$ and to $y$. As we see in the next section, this lets us evaluate the left-hand side of (2.15) to obtain Theorem 2.1.

2.9. Proof of the main result. As defined in (2.2), we consider the functions $\hat{\psi} = \hat{\psi}(y, X) = \psi(y - X\hat{\beta})$ and $\hat{\beta} = \hat{\beta}(y, X)$ as functions of $(y, X) \in \mathbb{R}^n \times \mathbb{R}^{n \times p}$. At a point $(y, X)$ where these functions are Frechet differentiable, the statistician has access to the Jacobians and partial derivatives in (2.3). These two functions, $\hat{\psi}$ and $\hat{\beta}$ are the only functions of $(y, X)$ that we will consider; the hat in $\hat{\psi}, \hat{\beta}$ emphasize that these are functions of $(y, X)$.

In the proof, we argue conditionally on $\epsilon$ and consider functions of $X$ only, such as
\begin{equation}
\psi = \psi(y - X\hat{\beta}), \quad r = n^{-\frac{1}{2}}\psi = n^{-\frac{1}{2}}\psi(y - X\hat{\beta}), \quad h = \hat{\beta} - \hat{\beta} \quad \text{valued in } \mathbb{R}^n, \mathbb{R}^n \text{ and } \mathbb{R}^p \text{ respectively. Formally, } \psi : \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^n, \quad r : \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^n, \quad h : \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^p \text{ and we view the functions in (2.23) as functions of } X \text{ only while the noise } \epsilon \text{ is fixed. We may write } r = r(X) \text{ to recall that convention. We will denote their partial derivatives by } (\partial/\partial x_{ij}). \text{ With the above definitions, the function } \psi = \psi(X) \text{ is related to } \hat{\psi} = \hat{\psi}(y, X) \text{ by } \psi = \hat{\psi}(X\beta + \epsilon, X) \text{ so that if } \psi \text{ is Frechet differentiable at } (y, X) \text{ we have }
\end{equation}
\begin{equation}
\sqrt{n}(\partial/\partial x_{ij})r(X) = (\partial/\partial x_{ij})\psi(X) = [(\partial/\partial x_{ij})\hat{\psi}(y, X) + \beta_j (\partial/\partial y_j)\hat{\psi}(y, X)]
\end{equation}
\begin{equation}
= -\text{diag}(\psi')X\hat{A}e_j \hat{\psi}_i - Ve_i \beta_j - \beta_j)
\end{equation}
with $V \in \mathbb{R}^{n \times n}$ given by (2.22).

Proof of Theorem 2.1 under Assumption 2.3(i). Let us start with the proof under the strongly convex assumption Assumption 2.3(i). By the change of variable (2.12), we may assume that $\Sigma = I_p$ and $X$ has iid $N(0, 1)$ entries.

By Proposition 4.4 and (4.6) we have that the function $\rho(X)$ in (2.14) is $K$-Lipschitz where $K = (n^{-1/2}L_\ast)$ and $L_\ast = \max(1, \mu^{-1})$. The Frobenius norm of the Jacobian of a $K$-Lipschitz function $\mathbb{R}^{n \times p} \rightarrow \mathbb{R}^n$ is bounded above by the rank of the Jacobian times its squared operator norm, and the operator norm of the Jacobian is bounded from above by $K$. Thus the Frobenius norm of the Jacobian of $\rho$ satisfies $\sum_{i=1}^n \sum_{j=1}^p \|\partial \rho/\partial x_{ij}\|^2 \leq nK^2$ because the rank is at most $n$. We obtain that the quantity RHS in the right-hand side of (2.15) is bounded from above by
\begin{equation}
4\mathbb{E}[L_\ast^2] + \sqrt{p + n} + \mathbb{E}(\rho + \|X\|^2_{op})4L_\ast^{1/2}
\end{equation}
which is smaller than $\sqrt{nC_{14}(\gamma, \mu)}$ thanks to Lemma 6.1 to bound from above the expectation of $\|X\|^2_{op}$ for a random matrix with iid $N(0, 1)$ entries.
Writing $D = (\|\mathbf{h}\|^2 + \|\mathbf{r}\|^2)^{1/2}$ for the denominator, we have $\mathbf{r} = \mathbf{D}^{-1}\mathbf{r}$. Using (2.24) and the product rule $\frac{\partial}{\partial x_{ij}} \mathbf{r} = \mathbf{D}^{-1} \frac{\partial}{\partial x_{ij}} \mathbf{r} + \mathbf{r} \frac{\partial}{\partial x_{ij}} \mathbf{D}^{-1}$, the last term in the left-hand side of (2.15) equals

$$-2 \sum_{i=1}^{n} \sum_{j=1}^{p} \rho_i e_j^\top X^\top \frac{\partial \mathbf{r}}{\partial x_{ij}} = 2 \sum_{i=1}^{n} \sum_{j=1}^{p} \left[ \rho_i e_j^\top X^\top \operatorname{diag}(\psi^\prime) X \hat{\mathbf{A}} e_j + \rho_i e_j^\top X^\top \mathbf{V} e_j h_j \right] \frac{\partial (\mathbf{D}^{-1})}{\partial x_{ij}}$$

\[(2.26)\]

$$= 2 \mathbf{d}^\top \| \mathbf{r} \|^2 + 2 \mathbf{h}^\top \mathbf{V} \mathbf{r} \frac{\partial (\mathbf{D}^{-1})}{\partial x_{ij}} - 2 \sum_{i=1}^{n} \sum_{j=1}^{p} \rho_i e_j^\top X^\top \mathbf{r} \frac{\partial (\mathbf{D}^{-1})}{\partial x_{ij}}$$

thanks to $\hat{\psi}_i/(\sqrt{n}) = \rho_i$ and $\mathbf{d} = \sum_{j=1}^{p} e_j^\top X^\top \operatorname{diag}(\psi^\prime) X \hat{\mathbf{A}} e_j = \operatorname{Tr}[X^\top \operatorname{diag}(\psi^\prime) X \hat{\mathbf{A}}]$ for the first term. For the second term, since $\mathbf{V}$ is the Jacobian of $\hat{\psi}$ with respect to $y$, by Proposition 2.2 we have $\|\mathbf{V}\|_{\text{op}} \leq 1$. By the Cauchy-Schwarz inequality and using $\|\mathbf{r}\| \leq 1$, $\|\mathbf{h}\| \leq \mathbf{D}$, the absolute value of the second term is smaller than $2\|\mathbf{X}\|_{n^{-1/2}} \mathbf{D}^{-1}$. By the Cauchy-Schwarz inequality, the third term is smaller than $\|X^\top \mathbf{r}\| \|\mathbf{r}\| \left( \sum_{j=1}^{n} \sum_{j=1}^{p} (\frac{\partial (\mathbf{D}^{-1})}{\partial x_{ij}})^2 \right)^{1/2}$. Inequality (4.8) shows that the gradient of the map $\mathbf{D}^{-1} : \mathbb{R}^{n \times p} \to \mathbb{R}$ has Euclidean norm at most $n^{-1/2} L_s \mathbf{D}^{-1}$, that is, $\left[ \sum_{i=1}^{n} \sum_{j=1}^{p} (\frac{\partial (\mathbf{D}^{-1})}{\partial x_{ij}})^2 \right]^{1/2} \leq n^{-1/2} L_s \mathbf{D}^{-1}$. Hence using $\|\mathbf{r}\| \leq 1$ and $\|\mathbf{r}\| \mathbf{D}^{-1} \leq 1$, the third term in (2.26) is bounded from above by $2\|\mathbf{X}\|_{n^{-1/2}} \mathbf{D}^{-1}$. In summary, for the last term on the left-hand side of (2.15),

\[(2.27)\]

$$\|2 \sum_{i=1}^{n} \sum_{j=1}^{p} \rho_i e_j^\top X^\top \frac{\partial \mathbf{r}}{\partial x_{ij}} + 2 \mathbf{d}^\top \| \mathbf{r} \|^2 \| \leq 2 \|\mathbf{X}\|_{n^{-1/2}} \mathbf{D}^{-1} + 2 L_s \|\mathbf{X}\|_{n^{-1/2}} \mathbf{D}^{-1}$$

which satisfies $\mathbb{E}[(2.27)] \leq C_{15}(\gamma, \mu)$ by Lemma 6.1. For the term $\sum_{j=1}^{n} (\sum_{i=1}^{n} \frac{\partial \mathbf{r}}{\partial x_{ij}})^2$ in the left-hand side of (2.15),

\[(2.28)\]

$$\frac{\operatorname{Tr}[\mathbf{V} h_j]}{\sqrt{n}} + \sum_{i=1}^{n} \frac{\partial \mathbf{r}_i}{\partial x_{ij}} = -\hat{\psi}^\top \operatorname{diag}(\psi^\prime) X \hat{\mathbf{A}} e_j + \sum_{i=1}^{n} \frac{\partial \mathbf{D}^{-1}}{\partial x_{ij}}$$

by (2.24), for any fixed $j \in [p]$. For the first term on the right-hand side we have $\sum_{j=1}^{n} \left( \frac{1}{\sqrt{n}} \hat{\psi}^\top \operatorname{diag}(\psi^\prime) X \hat{\mathbf{A}} e_j \right)^2 = \|\hat{\mathbf{A}} \|_{\text{op}}^2 ||\mathbf{X}||_{\text{op}}^2$. For the second term on the right-hand side of (2.28), by the Cauchy-Schwarz inequality $\sum_{j=1}^{p} \left[ \sum_{i=1}^{n} \frac{\partial \mathbf{D}^{-1}}{\partial x_{ij}} \right]^2 \leq \|\mathbf{r}\|_{n^{-1/2} \mathbf{D}^{-1}} \mathbf{D}^{-1} \leq n^{-1} L_s \mathbf{D}^{-1}$ since the norm of the gradient of $\mathbf{D}^{-1}$ satisfies $\left[ \sum_{i=1}^{n} \sum_{j=1}^{p} (\frac{\partial (\mathbf{D}^{-1})}{\partial x_{ij}})^2 \right]^{1/2} \leq n^{-1/2} L_s \mathbf{D}^{-1}$ again thanks to (4.8). Consequently, $\mathbf{a}, \mathbf{b} \in \mathbb{R}^p$ defined componentwise as

\[(2.29)\] $a_j = -\frac{\operatorname{Tr}[\mathbf{V} h_j]}{\sqrt{n}}, \quad b_j = \sum_{i=1}^{n} \frac{\partial \mathbf{r}_i}{\partial x_{ij}}$ satisfy $\| \mathbf{b} - \mathbf{a} \| \leq \|\mathbf{A}\|_{\text{op}} \|\mathbf{X}\|_{\text{op}} + n^{-1/2} L_s$.

For the difference of squares, $\|\|\mathbf{b}\|^2 - \|\mathbf{a}\|^2\| = \|\mathbf{b} - \mathbf{a}\|^2 + 2(\mathbf{b} - \mathbf{a})^\top \mathbf{a} \leq \|\mathbf{b} - \mathbf{a}\|^2 + 2\|\mathbf{a}\| \|\mathbf{b} - \mathbf{a}\|$. Next, $\|\mathbf{a}\|^2 \leq n^{-1} \|\mathbf{V}\|^2 \|\mathbf{h}\|^2 / D^2 \leq n$ since $\|\mathbf{h}\| \leq \mathbf{D}$ and $0 \leq \|\mathbf{V}\| \leq n$ by Proposition 2.2. Thus

\[(2.30)\]

$$\left( \sum_{i=1}^{n} \sum_{j=1}^{p} \frac{\partial \mathbf{r}_i}{\partial x_{ij}}^2 - \operatorname{Tr}[\mathbf{V}]^2 \|\mathbf{h}\|^2 \right) / n \mathbf{D}^2 \leq \left( \|\mathbf{A}\|_{\text{op}} \|\mathbf{X}\|_{\text{op}} + \frac{L_s}{\sqrt{n}} \right)^2 + \left( \|\mathbf{A}\|_{\text{op}} \|\mathbf{X}\|_{\text{op}} + \frac{L_s}{\sqrt{n}} \right)^2 \sqrt{n}$$

Using Lemma 6.1 and (2.20) again, $\mathbb{E}[(2.30)] \leq C_{16}(\gamma, \mu)$. An application of (2.15) combined with the bounds in expectation obtained for (2.27) and (2.30) thus provides $\mathbb{E} \|\mathbf{X}^\top \mathbf{r} \|^2 + (2\mathbf{d} - \mathbf{p}) \|\mathbf{p} \|^2 - \operatorname{Tr}[\mathbf{V}]^2 \|\mathbf{h}\|^2 \frac{1}{D^2 n} \leq C_{17}(\gamma, \mu) \sqrt{n}$ which is exactly Theorem 2.1 under Assumption 2.3(i).

We mention in passing that using the notation and the bound in (2.29), the first term in (2.16) satisfies

\[(2.31)\]

$$\left( \sum_{j=1}^{p} \rho_j^\top X e_j \sum_{i=1}^{n} \frac{\partial \mathbf{r}_i}{\partial x_{ij}} + \operatorname{Tr}[\mathbf{V}]^2 \|\mathbf{h}\| \sqrt{n} / \sqrt{n} \right) = \|\rho^\top X (\mathbf{b} - \mathbf{a}) \| \leq \|\mathbf{A}\|_{\text{op}} \|\mathbf{X}\|_{\text{op}}^2 + n^{-1/2} \|\mathbf{X}\|_{\text{op}}^2 L_s$$
so that $\mathbb{E}[\text{RHS}(2.31)] \leq C_{18}(\mu, \gamma)$ by Lemma 6.1 and (2.20).

\textbf{Proof of Theorem 2.1 under Assumption 2.3(ii).} If $\mu_{\rho} > 0$, by Proposition 2.2 and with the notation of Lemma 2.6, the matrix $V = \text{diag}(\psi') - \text{diag}(\psi') \hat{A} \hat{A}^\top \text{diag}(\psi')$ is symmetric psd. Let $(u_1, \ldots, u_q)$ be an orthonormal basis of $\ker(\text{diag}(\psi') \hat{A} \hat{A}^\top \text{diag}(\psi'))$ and note that $q \geq n - p$ since $X$ and the $n \times n$ matrix inside $\ker$ have rank at most $p$. Since $V$ is psd, $\text{Tr}[V] \geq \sum_{i=1}^q u_i^\top V u_i = \sum_{i=1}^q u_i^\top \text{diag}(\psi') u_i$. Since $\psi' \geq \mu_{\rho}$ by Assumption 2.3(ii), we obtain $\text{Tr}[V] \geq \mu_{\rho} q \geq \mu_{\rho} (n - p) \geq \mu_{\rho} (1 - \gamma)$ as desired.

The argument and notation are the same as in the previous proof. We apply (2.15) with only two notable differences. First, by Proposition 4.5, $L_*$ is now random and can be chosen (enlarging $L_*$ if necessary) as

\begin{equation}
(2.32) \quad L_* = C_{19}(\mu_{\rho}) \max(1, \|n^{-1/2}X\|_{\text{op}}) / \min(1, \phi_{\min}(\frac{1}{n} X^\top X)).
\end{equation}

The Jacobian of $\rho(X)$ has operator norm at most $2L_* n^{-1/2}$ by (4.6) and the gradient of $D^{-1}$ has Euclidean norm at most $L_* n^{-1/2}$ by (4.8). Second, we use the operator norm bound $\|A\|_{\text{op}} \leq \frac{1}{\mu_{\rho}} \phi_{\min}(\frac{1}{n} X^\top X)^{-1}$ by (2.20). Inequality (2.25) [upper bound on the quantity RHS in (2.15)], inequality (2.27) [upper bound on the negligible terms in (2.26)] and inequality (2.30) are still valid, and these three upper bounds are, in expectation, smaller than $C_{20}(\mu_{\rho}, \gamma) \sqrt{n}$ since by Lemmas 6.1 and 6.2 and the Cauchy-Schwarz inequality we have $\mathbb{E}[\max(1, \|n^{-1/2}X\|_{\text{op}}^k / \min(1, \phi_{\min}(\frac{1}{n} X^\top X)^k)] \leq C_{21}(\gamma, k, k')$ for any absolute constants $k, k'$; for our purpose we may take $k = 4, k' = 2$.

The proofs under Assumption 2.3(iii.a) and (iii.b) are more technical as the right-hand side of Corollary 2.5, (2.27) and (2.30) can only be controlled in a high-probability event $\Omega$. To overcome this problem, we use the argument detailed in the next section. The formal proofs of Theorem 2.1 under Assumption 2.3(iii.a) and (iii.b) are provided in Sections 10 and 11.

2.10. \textbf{Kirszbraun’s theorem: controlling derivatives outside high-probability events.} Under Assumption 2.3(i) and (ii), the proof of Theorem 2.1 leverages that for a fixed noise vector $\varepsilon$, the function $X \mapsto \rho(X)$ defined in (2.14) satisfies

\begin{equation}
(2.33) \quad \|\rho(X) - \rho(X')\| \leq n^{-1/2} L_* \|X - X'\|_F
\end{equation}

for some deterministic $L_* = C_{22}(\mu)$ under Assumption 2.3(i) and a random but integrable $L_*$ given by (2.32) under Assumption 2.3(ii). For the Lasso and Huber Lasso in Assumption 2.3(iii), we are only able to derive inequality (2.33) for $X, X' \in U_\varepsilon$ for some open set $U_\varepsilon \subset \mathbb{R}^{n \times p}$ such that the event $\Omega = \{X \in U_\varepsilon\}$ has $\mathbb{P}(\Omega) \to 1$. We use the following variant of Corollary 2.5 to prove Theorem 2.1 in such situations where the derivatives of $\rho(X)$ cannot be controlled in a small probability event $X \not\in U_\varepsilon$.

\textbf{Corollary 2.7.} Let $L > 0$ and $U \subset \mathbb{R}^{n \times p}$ be open. Assume that $X$ has iid $N(0, 1)$ entries, that $\rho : \mathbb{R}^{n \times p} \to \mathbb{R}$ is weakly differentiable and that $\|\rho(X)\| \leq 1$ and $\|\rho(X) - \rho(X')\| \leq L n^{-1/2} \|X - X'\|_F$ for any two $X, X' \in U$. Then for RHS $= L^2 + (1 + L) \sqrt{p + n}$ we have

\begin{equation}
(2.34) \quad \mathbb{E}\left[\mathbf{1}\{X \in U\}\|X^\top \rho - p\|_2^2 - p\|\rho\|_2^2 - \sum_{j=1}^p \left(\sum_{i=1}^n \frac{\partial \rho_i}{\partial x_{ij}}\right)^2 - 2 \sum_{i,j=1}^p \rho_i e_j^\top X^\top \frac{\partial \rho}{\partial x_{ij}}\right] \leq C_{23}\text{RHS},
\end{equation}

\begin{equation}
(2.35) \quad \mathbb{E}\left[\mathbf{1}\{X \in U\}\sum_{j=1}^p \rho_j e_j^\top X e_j \sum_{i=1}^n \frac{\partial \rho_i}{\partial x_{ij}} - \sum_{i,j=1}^p \left(\sum_{i=1}^n \frac{\partial \rho_i}{\partial x_{ij}}\right)^2 - \sum_{i,j=1}^p \rho_i e_j^\top X^\top \frac{\partial \rho}{\partial x_{ij}}\right] \leq C_{24}\text{RHS}.
\end{equation}

\textbf{Proof.} By Kirszbraun’s theorem, there exists $\overline{\rho} : \mathbb{R}^{n \times p} \to \mathbb{R}^n$ such that $\overline{\rho}(X) = \rho(X)$ for $X \in U$ and $\overline{\rho}$ is $n^{-1/2}L$-Lipschitz on the whole $\mathbb{R}^{n \times p}$. Applying Corollary 2.5 to $\overline{\rho}$, the right-hand sides of (2.15) and (2.16) for $\overline{\rho}$ are bounded from above by an absolute constant times $L^2 + \sqrt{p + n} + \ldots$
\[\mathbb{E}[p + \|X\|_{\text{op}}^2]^2 \leq L^2 \] since the Frobenius norm of the Jacobian of a Lipschitz map \(\mathbb{R}^{np} \rightarrow \mathbb{R}^n\) is bounded by \(n\) times the square of the Lipschitz constant. The left-hand side of (2.15) for \(\mathbf{p}\) is bounded from below by the left-hand side of (2.34) since \(I\{X \in U\} \leq 1\), hence (2.34) for \(\rho\) follows from (2.15) for \(\mathbf{p}\). Similarly, (2.35) for \(\rho\) follows from (2.16) for \(\mathbf{p}\). \(\square\)

Consequently, as long as (2.33) and \(\mathbb{P}(X \in U_\varepsilon) \rightarrow 1\) hold, and the remainder terms (2.30) and (2.27) are negligible for \(X \in U_\varepsilon\), the same algebra as in Section 2.8 can be used to derive a version of Theorem 2.1 that holds in the event \(\Omega = \{X \in U_\varepsilon\}\). This approach is used in Sections 10 and 11 for the formal proof of Theorem 2.1 under Assumption 2.3(iii.a) and (iii.b).

### 2.11. Approximation of the multiplicative factors in \(\hat{R}\) for arbitrary loss and penalty \((\rho, g)\).

For general penalty function, however, no closed form solution is available. Still, it is possible to approximate the multiplicative factors appearing in \(\hat{R}\) using the following Monte Carlo scheme. Since \(\text{Tr}[(\partial/\partial y)\hat{\psi}] = \text{Tr}[(\partial/\partial y)X\hat{\beta}]\) are the divergence of the vector fields \(y \mapsto \hat{\psi}\) and \(y \mapsto X\hat{\beta}\) respectively, we can use the following Monte Carlo approximation of the divergence of a vector field, which was suggested at least as early as [35], and for which accuracy guarantees are proved in [6].

Let \(F : \mathbb{R}^n \rightarrow \mathbb{R}^n\) be a vector field, and let \(z_k, k = 1, \ldots, m\) be iid standard normal random vector in \(\mathbb{R}^n\). Then for some small scale parameter \(a > 0\), we approximate the divergence of \(F\) at a point \(y \in \mathbb{R}^n\) by

\[
\text{div } F(y) = \frac{1}{m} \sum_{k=1}^m a^{-1} z_k^\top [F(y + az_k) - F(y)].
\]

Computing the quantities \(F(y + az_k)\) at the perturbed response vector \(y + az_k\) for \(F(y) = X\hat{\beta}\) or \(F(y) = \psi(y - X\hat{\beta})\) requires the computation of the \(M\)-estimator \(\hat{\beta}(y + az_k, X)\) at the perturbed response. If \(\hat{\beta}(y, X)\) has already been computed as a solution to (1.2) by an iterative algorithm, one can use \(\hat{\beta}(y, X)\) as a starting point of the iterative algorithm to compute \(\hat{\beta}(y + az_k, X)\) efficiently, since for small \(a > 0\) and by continuity, \(\hat{\beta}(y, X)\) should provide a good initialization. We refer to [6] for an analysis of the accuracy of this approximation.

Hence, even in situations where no closed form expressions for the Jacobians \((\partial/\partial y)\hat{\psi}\) and \((\partial/\partial y)X\hat{\beta}\) are available, the estimate \(\hat{R}\) of the out-of-sample error of the \(M\)-estimator \(\hat{\beta}\) can be used by replacing the divergences \(\text{Tr}[(\partial/\partial y)\hat{\psi}]\) and \(\hat{d}\) by their Monte Carlo approximations. Figure 1 illustrates the use of this Monte Carlo scheme by showing boxplots \(\hat{R}\) and its target \(\|\Sigma^{1/2}(\hat{\beta} - \beta)\|^2\) over 10 repetitions for the nuclear norm penalty over a range of tuning parameters.

Although this approximation scheme induces some computational overhead as it requires computation of several \(\hat{\beta}(y + az_k, X)\), we stress that this approximation scheme is not needed for the \(\ell_1\) and Elastic-Net penalty since explicit formulae are available (cf. Propositions 2.3 and (2.4)). For these two commonly used penalty functions the computational burden of computing \(\hat{d}\) and \(\text{Tr}[(\partial/\partial y)\hat{\psi}]\) is negligible.

### 2.12. Simulation study.

#### 2.12.1. Huber Lasso.

We illustrate the above result with a short simulation study. For given tuning parameters \(\lambda, \lambda_* > 0\), the \(M\)-estimator \(\hat{\beta}\) is the Huber Lasso estimator (1.2) with loss \(\rho\) and penalty \(g\) given in Proposition 2.4, and the estimate \(\hat{R}\) is given by (2.11). We set \(n = 1001, p = 1000, \Sigma = I_p\) and \(\beta\) has 100 nonzero coefficients all equal to 10\(p^{-1/2}\). The components of \(\varepsilon\) are iid with \(t\)-distribution with 2 degrees-of-freedom (so that the variance of each component does not exist). Define the sets \(\Lambda = \{0.1n^{-1/2}(1.5)^k, k = 0, \ldots, 15\}\) and \(\Lambda_* = \{0.1n^{-1/2}(1.5)^k, k = 0, \ldots, 8\}\). For each \((\lambda, \lambda_*)\) in the discrete grid \(\Lambda \times \Lambda_*\), the estimator \(\hat{R}\), its target \(\|\Sigma^{1/2}(\hat{\beta} - \beta)\|^2\) and the relative error
value 3 5

Section 2.6). These inaccurate estimations for low values for (λ,λ) are computed for each value of λ. The function mat : Rp → R^{20×25} maps Rp to matrices of size 20 × 25 so that the inverse map is the usual vectorization operator. For the true β, mat(β) is rank 3.

The Monte Carlo scheme of Section 2.11 is used to compute df with a = 0.01 and m = 100. The full simulation setup is described in Section 2.12.2.

|1 − ̂R|/||Σ^{1/2}(̂β − β)||^2| are reported, over 100 repetitions, in the boxplots in Figure 2. Figure 2 provides also a heatmap of the average of ̂R and ||Σ^{1/2}(̂β − β)||^2 over the same 100 repetitions.

The plots show that the estimate ̂R accurately estimates ||Σ^{1/2}(̂β − β)||^2 across the grid Λ × Λ∗, at the exception of the lowest value of the Huber loss parameter λ∗ coupled with the two lowest values for the penalty parameter λ as seen on the left of the top left boxplot in Figure 2. These low values for (λ, λ∗) lead to small values for (|̂R| − |S|)^2 in the denominator of (2.11). This provides additional evidence that ̂R should not be trusted for low values of Tr[|∂y/∂y|̂ψ]^2/n^2 (cf. Section 2.6). These inaccurate estimations for low values for (λ, λ∗) do not contradict the theoretical results, as the proof of Theorem 2.1 bounds from above (Tr[(∂y/∂y|̂ψ)/n^2]|̂R − ||Σ^{1/2}h||^2| = (|̂R| − |S|)^2 close to 0. Furthermore, Figure 2 suggests that the estimate ̂R is accurate for (λ, λ∗) smaller than the values (λ, λ∗) required in Assumption 2.3(iii.b). This suggests that the validity of ̂R may hold for smaller tuning parameters than those required by Assumption 2.3(iii.a) or (iii.b). The recent result from [13] also confirms this: The theory for the Lasso [13] holds for any constant tuning parameter λ, with no assumption of the form λ ≥ σλ∗ as required in Assumption 2.3(iii.a) for the proofs in the present paper.

2.12.2. Square loss and nuclear norm penalty. A second simulation study is provided with the square loss ρ(u) = u^2/2 and nuclear norm penalty. With n = 400, p = 500, a linear isomorphism mat : Rp → R^{20×25} is fixed so that the inverse map is the usual vectorization operator. The true β is such that mat(β) has iid N(0,1) entries in the first three columns and zeros in the remaining columns so that mat(β) is rank 3. The covariance matrix Σ ∈ Rp is defined as Σ = W/(5p) where W is a Wishart matrix with identity covariance and 5p degrees of freedom; Σ is generated once and is the same across the repetitions. The noise ε has iid N(0,2) entries. For 10 repetitions, (y, X) are generated and M-estimators with penalty proportional to the nuclear norm, g(b) = λ||mat(b)||^2_nuc, are computed for each value of λ in {0.5 · 1.3^k n^{-1/2}, k = 0, 1, 2, ..., 14}. For each λ, the estimate df is computed with the Monte Carlo scheme of Section 2.11 with a = 0.01 and m = 100 and used to
Figure 2. Boxplots over 100 repetitions of the out-of-sample error $\|\Sigma^{1/2}(\hat{\beta} - \beta)\|^2$ for the Huber Lasso with parameters $(\lambda, \lambda_1)$, the estimate $\hat{R}$ in (2.11) and the relative error $|1 - \hat{R}/\|\Sigma^{1/2}(\hat{\beta} - \beta)\|^2|$. The heatmap below displays the average over the same 100 repetitions of $\hat{R}$ (Left) and $\|\Sigma^{1/2}(\hat{\beta} - \beta)\|^2$ (Right). The experiment is described in Section 2.12.
3. Square loss

Throughout this section $\rho(u) = u^2/2$ in (1.2) so that $\hat{\beta}$ is the regularized least-squares

$$\hat{\beta}(y, X) = \arg \min_{b \in \mathbb{R}^p} \left( \|Xb - y\|^2/(2n) + g(b) \right).$$

for some convex penalty $g : \mathbb{R}^p \to \mathbb{R}$. Here $\psi(u) = \rho'(u) = u$, $\text{diag}(\psi') = I_n$ so that $\hat{\psi} = \psi(y - X\hat{\beta})$, $\text{Tr}((\partial/\partial y)\hat{\psi})$ are simply given by

$$\hat{\psi} = y - X\hat{\beta}, \quad \text{Tr}[V] = \text{Tr}[(\partial/\partial y)\hat{\psi}] = n - df,$$

i.e., $\hat{\psi}$ is the vector of residuals. In regression or sequence model with Gaussian noise, the quantity $df$ was introduced in [41] where Stein’s Unbiased Estimate (SURE) was developed, showing that $\mathbb{E}||X(\hat{\beta} - \beta)||^2 = \mathbb{E}[\text{SURE}]$ where $\text{SURE} = ||y - X\beta||^2 + 2\sigma^2\hat{df} - \sigma^2n$ when $\varepsilon \sim N(0, \sigma^2 I_n)$ under mild differentiability and integrability assumptions. Numerous works followed with the goal to characterize the quantity $\hat{df}$ for estimators of interest, see for instance [53, 46, 31, 23] for the Lasso and the Elastic-Net, [47] for the Group-Lasso, [36] for Slope and submodular regularizers, [14] for projection estimators, among others. A surprise of the present paper is that for general penalty functions, $\hat{df}$ is not only useful to estimate the in-sample error in $\mathbb{E}||X(\hat{\beta} - \beta)||^2 = \mathbb{E}[\text{SURE}]$, but also the out-of-sample error $||\Sigma^{1/2}(\hat{\beta} - \beta)||^2$. Furthermore, $\mathbb{E}||X(\hat{\beta} - \beta)||^2 = \mathbb{E}[\text{SURE}]$ requires normality of $\varepsilon$ while the estimate $\hat{R}$ of the present paper rely on the normality of $X$ but not that of $\varepsilon$.

3.1. Estimation of the noise level and generalization error. The simple algebraic structure of the square loss allows us to provide generic estimators of the noise level $\sigma^2$ and the generalization error $\sigma^2 + \|\Sigma^{1/2}h\|^2$, assuming that the components of $\varepsilon$ are iid with mean zero and variance $\sigma^2$. The quantity $\sigma^2 + \|\Sigma^{1/2}h\|^2$ can be seen as the generalization error, since $\sigma^2 + \|\Sigma^{1/2}h\|^2 = \mathbb{E}[(x_{\text{new}}^\top \hat{\beta} - y_{\text{new}})^2|(y, X)]$ where $(x_{\text{new}}^\top, y_{\text{new}})$ is independent of $(X, y)$ with the same distribution as any row of $(X, y) \in \mathbb{R}^n \times (p+1)$.

When the components of $\varepsilon$ are assumed iid, mean-zero with variance $\sigma^2$, the convergence $||\varepsilon||^2/n \to \sigma^2$ holds almost surely by the law of large numbers, and $||\varepsilon||^2/n - \sigma^2 = O_P(n^{-\frac{1}{2}})$ by the central limit theorem if the fourth moment of the entries of $\varepsilon$ is uniformly bounded as $n, p \to +\infty$. We may thus consider the estimation targets $\sigma^2 \overset{\text{def}}{=} ||\varepsilon||^2/n$ and $\sigma^2 + ||\Sigma^{1/2}h||^2$ for the noise level and generalization error, respectively. Results for $\sigma^2$ and $\sigma^2 + ||\Sigma^{1/2}h||^2$ can be deduced up to an extra additive error term of order $||\varepsilon||^2/n - \sigma^2$ which converges to 0 almost surely and that satisfies $||\varepsilon||^2/n - \sigma^2 = O_P(n^{-\frac{1}{2}})$ under the uniformly bounded fourth moment assumption on the components of $\varepsilon$. Define

$$\hat{\sigma}^2 = (n - \hat{df})^{-2}||y - X\hat{\beta}||^2n,$$

$$\hat{R} = (n - \hat{df})^{-2}\{||y - X\hat{\beta}||^2(2\hat{df} - p) + ||\Sigma^{-1/2}X^\top(y - X\hat{\beta})||^2\},$$

$$\hat{\sigma}^2 = (n - \hat{df})^{-2}\{||y - X\hat{\beta}||^2(n - (2\hat{df} - p)) - ||\Sigma^{-1/2}X^\top(y - X\hat{\beta})||^2\}.$$ 

**Theorem 3.1.** Let Assumption 2.2 be fulfilled. Set $\rho(u) = u^2/2$ (square loss) and assume that one of Assumption 2.3(i), (ii) or (iii) is fulfilled. Then almost surely

$$\left|\left|\Sigma^{1/2}h\right|^2 + \sigma^2 \right| - \hat{\sigma}^2 \leq (1 - \hat{df}/n)^{-2}(||y - X\hat{\beta}||^2/n + \left|\left|\Sigma^{1/2}h\right|^2\right|\text{Rem}_*$,$$

$$\left|\left|\Sigma^{1/2}h\right|^2 - \hat{R} \right| \leq (1 - \hat{df}/n)^{-2}(||y - X\hat{\beta}||^2/n + \left|\left|\Sigma^{1/2}h\right|^2\right|\text{Rem}_*,$$

$$\left|\sigma^2 - \hat{\sigma}^2 \right| \leq (1 - \hat{df}/n)^{-2}(||y - X\hat{\beta}||^2/n + \left|\left|\Sigma^{1/2}h\right|^2\right|\text{Rem}_*,$$

where $\text{Rem}_*$ and $(1 - \hat{df}/n)^{-1}$ in the right-hand side satisfy
(i) $\mathbb{E}[\text{Rem}_*] \leq C_{25}(\gamma, \mu)n^{-1/2}$ and $(1 - \bar{d}f/n)^{-1} \leq 1 + \frac{1}{\mu \|X\Sigma^{-1/2}\|_{op}^2} a.s.$ under Assumption 2.3(i), so that $\mathbb{P}((1 - \bar{d}f/n)^{-1} \leq 1 + (\sqrt{\gamma} + 1 + t)/\mu) \geq 1 - \exp(-t^2/2)$.

(ii) $\mathbb{E}[\text{Rem}_*] \leq C_{26}(\gamma, \mu)n^{-1/2}$ and $(1 - \bar{d}f/n)^{-2} \leq (1 - \gamma)^{-2}$ a.s. under Assumption 2.3(ii).

(iii) $\mathbb{E}[I(\Omega)\text{Rem}_*] \leq C_{27}(\gamma, \varphi)n^{-1/2}$ and $(1 - \bar{d}f/n)^{-2} \leq C_{28}(\gamma, \varphi)$ in $\Omega$ for some event $\Omega$ of probability converging to one under Assumption 2.3(iii.a).

**Proof of Theorem 3.1 under Assumption 2.3(i).** First, apply the change of variable (2.12) as in the proof of Theorem 2.1. We apply inequality (2.16) to $\rho$ in (2.13). The quantity RHS is bounded from above in (2.25) while the three terms in the left-hand side of (2.16) satisfy the approximations (2.31), (2.30) and (2.27). This gives, by the triangle inequality,

$$
(3.4) \quad \mathbb{E} - \frac{\text{Tr}[V]}{nD^2} h^\top X^\top \rho - \frac{\text{Tr}[V]^2}{nD^2} \|h\|^2 + \bar{d}f \|\rho\|^2 \leq (2.25) + \mathbb{E}[(2.27) + (2.30) + (2.31)].
$$

where each term on the right-hand side denotes the upper bound of the corresponding numbered equation in the previous section. For the square loss $\psi$ is the identity so that $\rho = (D^2 - Xh)$ and $\text{Tr}[V] = n - \bar{d}f$. Using these identities for the first term, the quantity inside the absolute value in the left-hand side of (3.4) equals

$$
n\|\rho\|^2 - \frac{\text{Tr}[V]^2}{nD^2} \|h\|^2 - \frac{\text{Tr}[V]}{nD^2} \varepsilon^\top \rho = n\|\rho\|^2 - \frac{\text{Tr}[V]^2}{nD^2} (\|h\|^2 + \frac{1}{n}\|\varepsilon\|^2) + \text{Rem}
$$

where $\text{Rem} = (D^2 n)^{-1} \text{Tr}[V](\text{Tr}[V] - n\|\varepsilon\|^2 \varepsilon^\top (\varepsilon - Xh))$. By the triangle inequality,

$$
(3.5) \quad \mathbb{E} n\|\rho\|^2 - \frac{\text{Tr}[V]^2}{nD^2} (\|h\|^2 + \frac{1}{n}\|\varepsilon\|^2) \leq \mathbb{E}[\text{Rem}] + (2.25) + \mathbb{E}[(2.27) + (2.30) + (2.31)].
$$

Proposition 8.1 provides the bound $\mathbb{E}[\text{Rem}] \leq C_{29}(\gamma)\sqrt{n}$ while the other terms in the right-hand side have been shown to be smaller than $C_{30}(\gamma, \mu)\sqrt{n}$ in the proof of Theorem 2.1. If we define $\text{Rem}_*$ such that $n\text{Rem}_*$ equals the random variable inside the expectation in the left-hand side of (3.5), then the bound on the first line of (3.3) is satisfied and $\mathbb{E}[\text{Rem}_*] \leq C_{31}(\gamma, \mu)n^{-1/2}$. The desired bound on the second line in (3.3) follows as a special case of Theorem 2.1 for the square loss, for a different $\text{Rem}_*$ again satisfying $\mathbb{E}[\text{Rem}_*] \leq C_{32}(\gamma, \mu)n^{-1/2}$. The bound on the third line in (3.3) is obtained by taking the difference of the first two lines, where this third $\text{Rem}_*$ is the sum of the $\text{Rem}_*$ in the first line and the $\text{Rem}_*$ in the second line.

It remains to bound $(1 - \bar{d}f/n)^{-1}$. If $X$ is fixed and $\tilde{y}, \check{y}$ are two response vectors with respective M-estimator $\hat{\beta}, \tilde{\beta}$ multiplying by $(\beta - \tilde{\beta})$ the KKT conditions $X^\top(\check{y} - X\check{\beta}) \in \partial g(\check{\beta})$ and $X^\top(\tilde{y} - X\tilde{\beta}) \in \partial g(\tilde{\beta})$ and taking the difference, we find

$$
(3.6) \quad n(\partial g(\check{\beta}) - \partial g(\tilde{\beta}))^\top(\check{\beta} - \tilde{\beta}) + \|X(\check{\beta} - \tilde{\beta})\|^2 \geq (\check{y} - \tilde{y})^\top X(\check{\beta} - \tilde{\beta}).
$$

Since the infimum of $(\partial g(\check{\beta}) - \partial g(\tilde{\beta}))^\top(\check{\beta} - \tilde{\beta})$ is at least $\mu\|\Sigma^{1/2}(\check{\beta} - \tilde{\beta})\|^2$ by strong convexity of $g$, this proves that $(n\mu\|X\Sigma^{-1/2}\|_{op}^2 + 1)^{-1}\|X(\check{\beta} - \tilde{\beta})\|^2 \leq (\check{y} - \tilde{y})^\top X(\check{\beta} - \tilde{\beta})$ in $\Omega$. Thus $\check{y} \mapsto X\check{\beta}(\check{y}, X)$ is $L$-Lipschitz and the operator norm of $(\partial/\partial \check{y})X\check{\beta}$ is bounded by $L$ for $L = (n\mu\|X\Sigma^{-1/2}\|_{op}^2 + 1)^{-1} < 1$. Thus $\bar{d}f = \text{Tr}[(\partial/\partial \check{y})X\check{\beta}] \leq nL$ and $(1 - \bar{d}f/n)^{-1} \leq (1 - L)^{-1} = 1 + \frac{1}{\mu\|X\Sigma^{-1/2}\|_{op}^2}$. Lemma 6.1 thus completes the proof for the tail bound on $(1 - \bar{d}f/n)^{-1}$.

**Proof of Theorem 3.1 under Assumption 2.3(ii).** The algebra is the same, in particular (3.4)-(3.5) are still valid. The bound $\mathbb{E}[\text{Rem}] \leq C_{33}(\gamma)\sqrt{n}$ is valid by Proposition 8.1 (cf. (8.2)) while (2.25), (2.31), (2.30) and (2.27) are bounded from above by $C_{34}(\mu, \gamma)\sqrt{n}$ under Assumption 2.3(ii) as explained in the proof of Theorem 2.1. By Theorem 2.1 with $\mu = 1$ for the square loss, $1 - \bar{d}f/n \geq 1 - \gamma$ always holds.

The proof under Assumption 2.3(iii.a) uses the argument from Section 2.10 and is provided in Section 10. The main message from Theorem 3.1 is that $\check{R}$ is consistent as an estimate of the
of the out-of-sample error $\|\Sigma^{\frac{1}{2}}h\|^2$, the estimate $\hat{\tau}^2$ is consistent for the generalization error $\|\Sigma^{\frac{1}{2}}h\|^2 + \sigma^2$, and the estimate $\hat{\sigma^2}$ is consistent for the noise level $\sigma^2 = \|\varepsilon\|^2/n$.

These estimates were known for the unregularized Ordinary Least-Squares in [33], for the Lasso penalty with square loss in [1, 2, 37], and for $\hat{\beta} = 0$ in [18]. Apart from these works and the specific Lasso penalty, to our knowledge the above estimates for general convex penalty $g$ are new, so that Theorem 3.1 considerably extends the scope of applications of the estimates $\hat{\tau}$, $\hat{\sigma^2}$ to using arbitrary data distribution, the above estimates are valid when the rows of $X$ are iid $N(0, \Sigma)$ and penalties with $\tau, \zeta > 0$ such that residual norm $\|X\hat{\beta}\|/\sqrt{n}$ and penalties with $\|\Sigma^{1/2}h\|^2$ converge respectively to $\tau_\varepsilon$ and $\tau$ at a rate $O_P(n^{-c})$ for $c > 0$ in the sense

$$1 - \frac{df}{n} - \frac{\|y - X\hat{\beta}\|/\sqrt{n}}{(\sigma^2 + \|\Sigma^{1/2}h\|^2)^{1/2}} \leq \frac{1}{1 - df/n} \left(1 - \frac{df}{n}\right)^2 - \frac{\|y - X\hat{\beta}\|^2/n}{\sigma^2 + \|\Sigma^{1/2}h\|^2} = O_P(n^{-1/2})$$

using $|a - b| \leq \frac{1}{2}(|a^2 - b^2|)$ for any $a, b > 0$ for the inequality. In particular, if there exist deterministic constants $\tau, \zeta > 0$ such the residual norm $\|y - X\hat{\beta}\|/\sqrt{n}$ and error $\|\Sigma^{1/2}h\|$ converge respectively to $\tau_\varepsilon$ and $\tau$ at a rate $O_P(n^{-c})$ for $c > 0$ in the sense

$$\frac{\|y - X\hat{\beta}\|/\sqrt{n}}{\sigma^2 + \|\Sigma^{1/2}h\|^2} = \tau + O_P(n^{-c})$$

then $1 - df/n = \zeta + O_P(\max\{n^{-c}, n^{-1/2}\})$ by (3.7). Results of the form (3.8) and the constants $\tau, \zeta$ are typically characterized by the fixed-point equations discussed around (1.4), see the recent works [13, 34] and references therein. For the Lasso, [13, Theorems 5 and 7] proves (3.8) for $c = 1/4$ up to logarithmic factors, and if Assumption 2.3(iii) additionally holds then Corollary 3.2 and (3.7) provides $1 - df/n = \zeta + O_P(n^{-1/4})$. This improves upon the rate $1 - df/n - \zeta = O_P(n^{-1/6})$ obtained in Theorem 8 of the same work. The argument used in [37, 13] to connect $1 - df/n$ to the fixed-point solutions $(\tau, \zeta)$ relies on relating $df$ to the law of the empirical distribution of the subgradient $X^\top(y - X\hat{\beta})$. This relationship between $df$ and the empirical distribution of the subgradient is specific to the $\ell_1$ penalty of the Lasso, and, as far as we are aware, this technique does not extend to M-estimators (3.1) other than $\ell_1$-penalized ones. Corollary 3.2 and (3.7) show that the connection between $1 - df/n$ and the ratio $\|y - X\hat{\beta}\|^2/(n(\sigma^2 + \|\Sigma^{1/2}h\|^2))$ holds beyond $\ell_1$-penalized estimates.
We conclude by supplementing the simulation setup in Section 2.12.2 with the estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$. Boxplots of these estimates and their targets are provided in Figure 3. The quantity of approximation deteriorates for the smallest tuning parameters, which can be explained by the multiplicative factor $1 - \hat{d}f/n$ being close to 0. An interesting phenomenon is visible regarding the empirical variance of the estimate $\hat{\sigma}^2$: the smallest variances are obtained for the tuning parameters with the smallest out-of-sample error. Our theoretical results do not explain this observation; further investigation of this phenomenon is left for future work.

4. Derivatives of $M$-estimators

4.1. Lipschitz properties. Throughout the paper and the following propositions, the penalty $g : \mathbb{R}^p \to \mathbb{R} \cup \{+\infty\}$ and loss function $\rho : \mathbb{R} \to \mathbb{R}$ are assumed convex.

Proposition 4.1. Let $\rho$ be a loss function such that $\psi$ is $L$-Lipschitz, where $\psi = \rho'$. Then for any fixed design matrix $X \in \mathbb{R}^{n \times p}$, the mapping $y \mapsto \psi(y - X\hat{\beta})$ is $L$-Lipschitz.

Proof. Let $y, \tilde{y} \in \mathbb{R}^n$ be two response vectors, $\hat{\beta} = \hat{\beta}(y, X), \tilde{\beta} = (\tilde{y}, X)$ and $\psi = \psi(y - X\hat{\beta}), \tilde{\psi} = \psi(\tilde{y} - X\tilde{\beta})$. The KKT conditions read $X^T\psi \in n\partial g(\hat{\beta})$ and $X^T\tilde{\psi} \in n\partial g(\tilde{\beta})$ where $\partial g(\beta)$ denotes the subdifferential of $g$ at $\beta$. Multiplying by $\hat{\beta} - \tilde{\beta}$ and taking the difference of the two KKT conditions above, we find

$$
n(\partial g(\hat{\beta}) - \partial g(\tilde{\beta}))^T(\hat{\beta} - \tilde{\beta}) + \{(y - X\hat{\beta}) - (\tilde{y} - X\tilde{\beta})\}^T(\psi - \tilde{\psi})$$

$$
\geq (y - \tilde{y})^T(\psi - \tilde{\psi}) = (X(\hat{\beta} - \tilde{\beta}))^T(\psi - \tilde{\psi}) + \{(y - X\hat{\beta}) - (\tilde{y} - X\tilde{\beta})\}^T(\psi - \tilde{\psi}).$$

By the monotonicity of the subdifferential, $(\partial g(\hat{\beta}) - \partial g(\tilde{\beta}))^T(\hat{\beta} - \tilde{\beta}) \in [0, \infty)$. We now lower bound the second term in the first line for each term indexed by $i = 1, \ldots, n$. Since $\psi : \mathbb{R} \to \mathbb{R}$ is nondecreasing and $L$-Lipschitz, $\psi(u) - \psi(v) \leq L(u - v)$ holds for any $u > v$, as well as $(\psi(u) - \psi(v))^2 \leq L(u - v)(\psi(u) - \psi(v))$ since $\psi(u) - \psi(v) \geq 0$ by monotonicity. Applying this inequality for each $i$ to $u = y_i - x_i^T\hat{\beta}$ and $v = \tilde{y}_i - x_i^T\tilde{\beta}$, we obtain

$$L^{-1}\|\psi - \tilde{\psi}\|^2 \leq \{(y - X\hat{\beta}) - (\tilde{y} - X\tilde{\beta})\}^T(\psi - \tilde{\psi}) \leq (y - \tilde{y})^T(\psi - \tilde{\psi}).$$

The Cauchy-Schwarz inequality completes the proof.

Proposition 4.1 generalizes the result of [5] to general loss functions. The following proposition uses a variant of (4.1) to derive Lipschitz properties with respect to $(y, X)$. 

![Figure 3](image-url)  

**Figure 3.** Estimators $\hat{\sigma}^2, \hat{\tau}^2$ and their targets for the nuclear norm penalty simulation described in Section 2.12.2. The distribution of the entries of the noises $\varepsilon$ are iid $N(0, 2)$.
**Proposition 4.2.** Assume that ψ is L-lipschitz. Let \((y, X) \in \mathbb{R}^n \times \mathbb{R}^{n \times p}\) and \((\bar{y}, \bar{X}) \in \mathbb{R}^n \times \mathbb{R}^{n \times p}\) be fixed. Let \(\bar{\beta} = \bar{\beta}(y, X)\) be the estimator in (1.2) with observed data \((y, X)\) and let \(\bar{\beta} = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \rho(y_i - e_i^T \bar{X}b) + g(b)\), i.e., the same M-estimator as (1.2) with the data \((y, X)\) replaced by \((\bar{y}, \bar{X})\). Set \(\psi = \psi(y - X\beta)\) as well as \(\psi = \psi(\bar{y} - \bar{X}\bar{\beta})\). Then

\[
\begin{align*}
\mu \|\Sigma^{1/2}(\beta - \bar{\beta})\|^2 + \max \left(L^{-1}\|\psi - \psi\|^2, \mu\rho\|y - X\bar{\beta} - \{y - \bar{X}\bar{\beta}\}\|^2\right) &
\leq (\beta - \bar{\beta})^T (X - X^T) \psi + (\bar{y} + (X - \bar{X})\bar{\beta} - y)^T (\psi - \psi).
\end{align*}
\]

Consequently

(i) The map \((y, X) \mapsto (\beta(y, X), \hat{\psi}(y, X))\) is Lipschitz on every compact subset of \(\mathbb{R}^n \times \mathbb{R}^{n \times p}\) if \(\mu > 0\) as in Assumption 2.3(i).

(ii) The map \((y, X) \mapsto (\beta(y, X), \hat{\psi}(y, X))\) is Lipschitz on every compact subset of \(\{(y, X) \in \mathbb{R}^n \times \mathbb{R}^{n \times p} : \phi_\min(\Sigma^{-1/2} X^T X \Sigma^{-1/2}) > 0\}\) if \(\mu > 0\) as in Assumption 2.3(ii).

(iii) If \(X = X\) and \(\bar{y} = y\), we must have \(\psi = \hat{\psi}\). This means that if \(\beta\) and \(\bar{\beta}\) are two distinct solutions of the optimization problem (1.2), then \(\psi(\bar{y} - X\bar{\beta}) = \psi(y - X\beta)\) must hold.

**Proof.** The KKT conditions for \(\hat{\beta}\) and \(\bar{\beta}\) read \(X^T \psi \in n\partial g(\bar{\beta})\) and \(X^T \psi \in n\partial g(\bar{\beta})\). If \(D_g = (\beta - \bar{\beta})^T (\partial g(\beta) - \partial g(\bar{\beta}))\) then

\[
D_g + (\bar{y} - \bar{X}\bar{\beta} - y + X\beta)^T (\psi - \hat{\psi})
\]

\[
\geq (\beta - \bar{\beta})^T (X^T \psi - X^T \psi) + (\bar{y} - \bar{X}\bar{\beta} - y + X\beta)^T (\psi - \hat{\psi})
\]

\[
= (\beta - \bar{\beta})^T (X - X^T) \psi + (\bar{y} + (X - \bar{X})\bar{\beta} - y)^T (\psi - \hat{\psi}).
\]

Since for any real \(u > s\) inequality \((u - s)(\psi(u) - \psi(s)) \geq L^{-1}(\psi(u) - \psi(s))^2\) holds when \(\psi\) is L-Lipschitz and non-decreasing, the first line is bounded from below by \((n \inf D_g + L^{-1}\|\psi - \hat{\psi}\|^2)\).

If Assumption 2.3(ii) is satisfied for some \(\mu > 0\), we also have \((u - s)(\psi(u) - \psi(s)) \geq \mu(u - s)^2\) so that the first line is bounded from below by \(\mu\rho\|y - X\bar{\beta} - \{y - \bar{X}\bar{\beta}\}\|^2\). We also have inf \(D_g \geq \mu\|\Sigma^{1/2}(\beta - \bar{\beta})\|^2\) by monotonicity of the subdifferential and strong convexity of \(g\) with respect to \(\Sigma\). This proves (4.2).

For (i), by bounding from above the right hand side of (4.2) we find

\[
\min(\mu, L^{-1})\|\Sigma^{1/2}(\beta - \bar{\beta})\|^2 + \|\psi - \hat{\psi}\|^2_2/n \leq n^{-1/2}\|y - \bar{y}\| + n^{-1/2}\|X - \bar{X}\|\Sigma^{1/2}\|\psi\|_\infty(n^{-1/2}\|\psi\| + \|\Sigma^{1/2}\bar{\beta}\|).
\]

By taking a fixed \(X\), e.g., \(X = 0_{n \times p}\), this implies that the supremum \(S(K) = \sup_{(y, X) \in K}(\|\Sigma^{1/2}\bar{\beta}\| + n^{-1/2}\|\psi\|)\) is finite for every compact \(K\). If \((y, X), (\bar{y}, \bar{X}) \in K\) the right hand side is bounded from above by \(n^{-1/2}\|y - \bar{y}\| + n^{-1/2}\|X - \bar{X}\|\Sigma^{-1/2}\|\psi\|_\infty S(K)\) which proves that the map is Lipschitz on \(K\).

For (ii), we use that on the left hand side of (4.2),

\[
\|y - X\beta - \{y - \bar{X}\bar{\beta}\}\|^2 = \|X(\beta - \bar{\beta})\|^2 + 2[\bar{X}(-\bar{\beta} + \bar{\beta})]^T [y - \bar{y} + (\bar{X} - X)\bar{\beta}] + \|y - \bar{y} + (\bar{X} - X)\bar{\beta}\|^2.
\]

Combined with (4.2) this implies that

\[
\min \{\mu\rho\min(\Sigma^{-1/2} \bar{X}^T \bar{X} \Sigma^{-1/2}), L^{-1}\} \|\Sigma^{1/2}(\beta - \bar{\beta})\|^2 + \|\psi - \hat{\psi}\|^2_2
\]

\[
\leq (\beta - \bar{\beta})^T (X - X^T) \psi + (\bar{y} + (X - \bar{X})\bar{\beta} - y)^T (\psi - \hat{\psi}) - 2[\bar{X}(-\bar{\beta} + \bar{\beta})]^T [y - \bar{y} + (\bar{X} - X)\bar{\beta}].
\]

The same argument as in (i) applies on every compact where the eigenvalues of \(n^{-1/2}\bar{X} \Sigma^{-1/2}\) are bounded away from 0 and \(+\infty\). Finally, (iii) directly follows from (4.2).
4.2. Lipschitz properties for a given, fixed $\varepsilon$. In this subsection, $\varepsilon$ is fixed and we consider functions of $X \in \mathbb{R}^{n \times p}$ as defined in the following Lemma.

Lemma 4.3. Let $\varepsilon \in \mathbb{R}^n$ be fixed and $X, \tilde{X}$ be two design matrices. Define $\tilde{\beta} = \hat{\beta}(X\beta + \varepsilon, X)$ and $\tilde{\beta} = \hat{\beta}(\tilde{X}\beta + \varepsilon, \tilde{X})$, $\psi = \psi(\varepsilon + X\beta - X\tilde{\beta})$ and $\tilde{\psi} = \psi(\varepsilon + \tilde{X}\beta - \tilde{X}\beta)$ as well as $r = n^{-\frac{1}{2}}\psi$ and $\tilde{r} = n^{-\frac{1}{2}}\tilde{\psi}$. $h = \beta - \beta$ and $\tilde{h} = \beta - \tilde{\beta}$. Let also $D = (\|r\|^2 + \|\Sigma^{\frac{1}{2}}h\|^2)^{\frac{1}{2}}$ and $\tilde{D} = (\|\tilde{r}\|^2 + \|\Sigma^{\frac{1}{2}}\tilde{h}\|^2)^{\frac{1}{2}}$.

If for some constant $L_*$ and $\{X, \tilde{X}\} \subset \mathbb{R}^{n \times p}$

\[
(4.4) \quad (\|\Sigma^{\frac{1}{2}}(h - \tilde{h})\|^2 + \|r - \tilde{r}\|^2)^{\frac{1}{2}} \leq n^{-\frac{1}{2}}(\|X - \tilde{X}\|\Sigma^{-\frac{1}{2}}\|_{op}L_*(\|r\|^2 + \|\Sigma^{\frac{1}{2}}h\|^2)^{\frac{1}{2}}
\]

holds, then we also have the Lipschitz properties

\[
(4.5) \quad \|\Sigma^{\frac{1}{2}}(hD^{-1} - \tilde{h}\tilde{D}^{-1})\| \leq n^{-\frac{1}{2}}||X - \tilde{X}||\Sigma^{-\frac{1}{2}}||_{op}2L_*,
\]

\[
(4.6) \quad \|rD^{-1} - \tilde{r}\tilde{D}^{-1}\| \leq n^{-\frac{1}{2}}||X - \tilde{X}||\Sigma^{-\frac{1}{2}}||_{op}2L_*,
\]

\[
(4.7) \quad n^{-\frac{1}{2}}||\Sigma^{-\frac{1}{2}}(\frac{X^\top r}{D} - \frac{\tilde{X}^\top \tilde{r}}{\tilde{D}})|| \leq n^{-\frac{1}{2}}||X - \tilde{X}||\Sigma^{-\frac{1}{2}}||_{op}(1 + 2L_*||n^{-\frac{1}{2}}\tilde{X}\Sigma^{-\frac{1}{2}}||_{op}),
\]

\[
(4.8) \quad |D^{-1} - \tilde{D}^{-1}| \leq n^{-\frac{1}{2}}||X - \tilde{X}||\Sigma^{-\frac{1}{2}}||_{op}L_*\tilde{D}^{-1}.
\]

Proof of Lemma 4.3. Assume that $\Sigma = I_p$ without loss of generality, by performing the variable change (2.12) if necessary. By the triangle inequality, $\|hD^{-1} - \tilde{h}\tilde{D}^{-1}\| \leq \|h\|D^{-1} - \tilde{D}^{-1}| + D^{-1}\|h - \tilde{h}\|$. Then $D^{-1}\|h - \tilde{h}\| \leq n^{-\frac{1}{2}}\|X - \tilde{X}\|\Sigma^{-\frac{1}{2}}\|_{op}L_*$ for the second term by (4.4). For the first term, $\|h\|D^{-1} - \tilde{D}^{-1} \leq D^{-1}|D - \tilde{D}| \leq D^{-1}||r - \tilde{r}||^2 + \|h - \tilde{h}\|^2)^{\frac{1}{2}}$ by the triangle inequality, and another application of (4.4) provides (4.5). The exact same argument provides (4.6) since the roles of $h$ and $r$ are symmetric in (4.4). For (4.7), we use

\[
\|X^\top rD^{-1} - \tilde{X}^\top \tilde{r}\tilde{D}^{-1}\| \leq \|X - \tilde{X}\|\Sigma^{-\frac{1}{2}}\|_{op}||r||D^{-1} + \|\tilde{X}\|\Sigma^{-\frac{1}{2}}\|_{op}||rD^{-1} - \tilde{r}\tilde{D}^{-1}||.
\]

Combined with (4.6) and $||r||D^{-1} \leq 1$, this provides (4.7). For the fourth inequality, by the triangle inequality $|D^{-1} - \tilde{D}^{-1}| \leq (D\tilde{D})^{-1}|D - \tilde{D}| \leq n^{-\frac{1}{2}}\|X - \tilde{X}\|\Sigma^{-\frac{1}{2}}\|_{op}L_*\tilde{D}$ thanks to (4.4).

\[\square\]

Proposition 4.4. Let Assumption 2.1 and Assumption 2.3(i) be fulfilled. Consider the notation of Lemma 4.3 for $X, \psi, r, h$ and $\tilde{X}, \tilde{\psi}, \tilde{r}, \tilde{h}$. Then by (4.2) we have

\[
\mu||\Sigma^{\frac{1}{2}}(h - \tilde{h})||^2 + ||r - \tilde{r}||^2 = \mu||\Sigma^{\frac{1}{2}}(\beta - \tilde{\beta})||^2 + ||\psi - \tilde{\psi}||/n
\]

\[
\leq \left[\frac{\|\tilde{h} - h\|^\top (\tilde{X} - X)^\top \psi + h^\top (X - \tilde{X})^\top (\tilde{\psi} - \psi)\right]/n
\]

\[
\leq n^{-\frac{1}{2}}\|\Sigma^{-\frac{1}{2}}(\tilde{h} - h)\|_{op}(\|\Sigma^{\frac{1}{2}}(\tilde{h} - h)\|^2 + ||\tilde{r} - r||^2)^{\frac{1}{2}}(\|r||^2 + \|\Sigma^{\frac{1}{2}}h\|^2)^{\frac{1}{2}}.
\]

Hence (4.4) holds for $L_* = \max(\mu^{-1}, 1)$ and all $X, \tilde{X} \in \mathbb{R}^{n \times p}$.

Proof. This follows by (4.2) with $\tilde{y} = \varepsilon + \tilde{X}\beta$ and $y = \varepsilon + X\beta$. The last inequality in (4.9) is due to the Cauchy-Schwarz inequality. Inequality (4.4) with the given $L_*$ is obtained by dividing by $(||r - \tilde{r}||^2 + \|\Sigma^{\frac{1}{2}}(h - \tilde{h})||^2)^{\frac{1}{2}}$.

\[\square\]

Proposition 4.5. Let Assumption 2.1 and Assumption 2.3(ii) be fulfilled. Consider the notation of Lemma 4.3 for $X, \psi, r, h$ and $\tilde{X}, \tilde{\psi}, \tilde{r}, \tilde{h}$. Then

\[
\min(1, \mu\phi_{min}(\Sigma^{-\frac{1}{2}}(h - \tilde{h})) \max\left(\|r - \tilde{r}\|, \|\Sigma^{\frac{1}{2}}h\|\right)
\]

\[
\leq n^{-\frac{1}{2}}\|\Sigma^{-\frac{1}{2}}(\tilde{h} - h)\|_{op}\|r\| + \|\Sigma^{\frac{1}{2}}\tilde{h}\|((1 + 2\mu||n^{-\frac{1}{2}}\tilde{X}\Sigma^{-\frac{1}{2}}||_{op})).
\]

Hence (4.4) holds with $L_* = \max(1, \mu\phi_{min}(\Sigma^{-\frac{1}{2}}\tilde{X}^\top \tilde{X}\Sigma^{-\frac{1}{2}})^{-1}6\max(1, 2\mu||n^{-1/2}\tilde{X}\Sigma^{-1/2}||_{op})$ for all $X, \tilde{X} \in \mathbb{R}^{n \times p}$.
Proof. By (4.2) we have
\[
\max(\|r - \bar{r}\|^2, \mu_p \|X h - \bar{X} h\|^2 / n) \leq \left[ (\bar{h} - h)^T (\bar{X} - X)^T \psi - h^T (X - \bar{X})^T (\psi - \psi) \right] / n.
\]
We also have \(\|X h - \bar{X} h\|^2 = \|X (h - \bar{h})\|^2 + 2 (X (h - \bar{h}))^T (X - \bar{X}) h + \|X - \bar{X}\|^2\) so that the previous display implies
\[
\max(\|r - \bar{r}\|^2, \mu_p \|X (h - \bar{h})\|^2 / n)
\]
\[
\leq \left[ (\bar{h} - h)^T (\bar{X} - X)^T \psi - h^T (X - \bar{X})^T (\psi - \psi) - 2 \mu_p (X (h - \bar{h}))^T (X - \bar{X}) h \right] / n
\]
and the conclusion holds by the Cauchy-Schwarz inequality and properties of the operator norm. □

5. GRADIENT IDENTITIES

Corollary 5.1. Let the setting and assumptions of Proposition 4.2 be fulfilled. If \(\bar{y} = y + \hat{\beta}_j v \) and \(\bar{X} = X + v e_j^T\) for any direction \(v \in \mathbb{R}^n\) with \(v^T \psi = 0\) and index \(j \in [p]\), then \(\bar{y} = \psi\) and the solution \(\hat{\beta}\) of the optimization problem (1.2) is also solution of the same optimization problem with \((y, X)\) replaced by \((\bar{y}, \bar{X})\). If additionally \(\mu > 0\), then \(\hat{\beta} = \hat{\beta}\) must hold.

Proof. The right-hand side of (4.2) is 0 for the given \(\bar{y} - y\) and \(\bar{X} - X\). This proves that \(\hat{\psi} = \psi\). Furthermore, the KKT conditions for \(\hat{\beta}\) read \(X^T \psi = n \partial g(\hat{\beta})\), and we have \(X^T \hat{\psi} = \hat{X}^T \psi\), and \(\psi = \psi(y - X \hat{\beta}) = \psi(\bar{y} - \bar{X} \hat{\beta})\). This implies that \(X^T \psi(y - X \hat{\beta}) \in n \partial g(\hat{\beta})\) so that \(\hat{\beta}\) is solution to the optimization problem with data \((\bar{y}, \bar{X})\), even if \(\mu = 0\). The claim \(\hat{\beta} = \hat{\beta}\) for \(\mu > 0\) follows by unicity of the minimizer of strongly convex functions. □

Proof of Lemma 2.6. Existence of the partial derivatives of \(\hat{\psi}\) and \(\hat{\beta}\) at \((y^0, X^0)\) is granted by the assumption of Frechet differentiability. If \(\hat{\psi}\) is continuously differentiable, the chain rule (2.21) holds. We now compute the directional derivatives. To this end, let \((\bar{y}, \bar{X}) \in \mathbb{R}^{n \times (1+p)}\) representing a perturbation direction (e.g., take \((\bar{y}, \bar{X}) = (e_t, 0_{n \times p})\) for the partial derivative in (2.19) or \((\bar{y}, \bar{X}) = (0_n, e_j e_j^T)\) for the partial derivative in (2.18)). For \(t \in \mathbb{R}\), let \((y(t), X(t)) = (y^0 + t \bar{y}, X^0 + t \bar{X})\) and \(b(t) = \beta(y(t), X(t))\). Set also \(\psi(t) = \psi(y(t) - X(t) b(t))\) where as usual \(\psi = \rho'\) acts componentwise. The KKT conditions at \(t = 0\) yield \(X(t)^T \psi(t) \in n \partial g(b(t))\) and \(X(0)^T \psi(0) \in n \partial g(b(0))\). Multiplying the difference of these KKT conditions by \((b(t) - b(0))\) and using the strong convexity of \(g\) with respect to \(\Sigma\), we find
\[
n \mu \|\Sigma^{1/2} (b(t) - b(0))\|^2 \leq (b(t) - b(0))^T [X(t)^T \psi(t) - X(0)^T \psi(0)] .
\]
Denote by \(\psi'(0)\) the derivatives at \(t = 0\). By the product rule \(\frac{d}{dt} X(t)^T \psi(t) |_{t=0} = X'(0)^T \psi'(0) + X^0 T \psi'(0)\) and by the chain rule \(\psi'(0) = D^0 \psi(y'(0) - X'(0) b(0) - X(0) b'(0))\) where \(D^0 = \text{diag} (\psi''(\psi'))\). Dividing by \(t^2\) and taking the limit \(t \to 0\) in the previous display and moving \(b'(0)^T D^0 X(0) b'(0)\) to the left-hand side gives
\[
n \mu \|\Sigma^{1/2} b'(0)\|^2 + \|D^0 X(0) b'(0)\|^2 \leq b'(0)^T [X'(0)^T \psi'(0) + X^0 T D^0 (y'(0) - X'(0) b(0) - X(0) b'(0))] .
\]
By definition of Frechet differentiability, the mapping \(\bar{B} : (\bar{y}, \bar{X}) \mapsto \Sigma^{1/2} b'(0)\) appearing in the left-hand side is a linear map \(\bar{B} : \mathbb{R}^n \times \mathbb{R}^{n \times p} \to \mathbb{R}^p\). The mapping \(\mathcal{L} : (y, X) \mapsto \Sigma^{-1/2} [X^T \psi'(0) + X^0 T D^0 (y - X^0 T \beta)]\) appearing on the right-hand side is also a linear map. Since \(\Sigma\) and the matrix inside \(\phi_{\min}(\cdot)\) in (2.20) are positive definite, \(\mathcal{L}(\bar{y}, \bar{X}) = 0_p\) implies \(b'(0) = 0_p\). Two linear mappings \(\mathcal{L}\) and \(\bar{B}\) from \(\mathbb{R}^{n \times p}\) to \(\mathbb{R}^p\) have ker\(\mathcal{L} \subset \ker\bar{B}\) if and only if there exists a matrix \(M\) with \(\ker(M) = \text{Image}(\mathcal{L})\) such that \(\bar{B} = M \mathcal{L}\). This proves the existence of \(\hat{A}(y^0, X^0)\) in (2.18)-(2.19) by taking \(\hat{A}(y^0, X^0) = \Sigma^{-1/2} M \Sigma^{-1/2}\). If \(u \in \mathbb{R}^p\) has unit norm and is a right singular vector associated with the largest singular value of \(M\) then \(\|M\|_{op} = \|Mu\|\) and \(u \in \ker(M)^\perp\).
Since \( \ker(M)^\perp \subset \text{Image}(\mathcal{L}) \) we can find \((y, \hat{X})\) such that \( u = \mathcal{L}(y, \hat{X}) \). Then previous display then yields \( f_{\min} \|Mu\|^2 \leq u^\top Mu \) where \( f_{\min}^{-1} \) is the right-hand side of (2.20). This provides \( \|M\|_{op} = \|Mu\| \leq f_{\min}^{-1} \) and concludes the proof of (2.20) since \( M = \Sigma^{1/2} \hat{A}(y^0, X^0) \Sigma^{1/2} \).

The second claim, where \( \psi \) is only assumed to be 1-Lipschitz, requires the chain rule (2.21) to hold for almost \((y^0, X^0)\) in \( U \). The validity of the chain rule (2.21) boils down to the chain rule for

\[ \psi \circ u_i \quad \text{where} \quad u_i : U \to \mathbb{R}, \quad (y, X) \mapsto u_i(y, X) = y_i - x_i^\top \beta(y, X) \]

for all \( i \in [n] \). Since \( \psi : \mathbb{R} \to \mathbb{R} \) is Lipschitz and \( u_i \) is Lipschitz in \( U \), \([52, \text{Theorem } 2.1.11]\) implies that \( (\partial/\partial y_i)^\hat{\psi}_i(y, X) = \psi'(u_i(y, X))((\partial/\partial y_i)u_i(y, X)) \) almost everywhere in \( U \). (This version of the chain rule is straightforward at points \((y, X)\) where \( \psi'(u_i(y, X)) \) and \((\partial/\partial y_i)u_i(y, X) \) both exist, as well as at points \((y, X)\) where \((\partial/\partial y_i)u_i(y, X) = 0 \) thanks to \( t^{-1}|\hat{\psi}(y + te_i, X) - \hat{\psi}(y, X)| \leq Mt^{-1}|u_i(y + te_i, X) - u_i(y, X)| \) in which case \((\partial/\partial y_i)^\hat{\psi}_i(y, X) = 0 \) and \( \psi'(u_i(y, X)) \) need not exist. The non-trivial part of the argument in \([52, \text{Theorem } 2.1.11]\) is to prove that the set \( \{(y, X) \in U : \psi'(u_i(y, X)) \text{ fails to exist and } (\partial/\partial y_i)u_i(y, X) \neq 0 \} \) has Lebesgue measure 0.)

6. Inequalities for Functions of Standard Multivariate Normals

This section provides several useful tail bound and moment inequalities for functions of a matrix with iid \( N(0, 1) \) entries, including the proof of Proposition 6.5.

**Lemma 6.1.** Let \( \gamma > 0 \). If \( p/n \leq \gamma \) and \( G \in \mathbb{R}^{n \times p} \) has iid \( N(0,1) \) entries then the tail bound

\[ \mathbb{P}(\|G\|_{op} > \sqrt{n} + \sqrt{p} + t) \leq \Phi(-t) \leq e^{-t^2/2} \]

holds where \( \Phi \) is the standard normal CDF. As a consequence \( \mathbb{E}[\|n^{-1/2}G\|_{op}^k] \leq C_{35}(k, \gamma) \) for any integer \( k \geq 1 \).

The above tail bound is given in \([17, \text{Theorem II.13}]\) and the moment bound \( \mathbb{E}[\|n^{-1/2}G\|_{op}^k] \leq C_{36}(k, \gamma) \) is obtained by integrating the tail bound. The next result is well known and follows from \([24]\) as explained in \([7, \text{Proposition A.1}]\) among others.

**Lemma 6.2** (Negative moments). Let \( \gamma \in (0, 1) \). If \( p/n \leq \gamma \) and \( G \in \mathbb{R}^{n \times p} \) has iid \( N(0,1) \) entries then \( \mathbb{E}[\phi_{\min}(\frac{1}{n}G^\top G)^{-k}] \leq C_{37}(k, \gamma) \) for any integer \( k \geq 1 \).

**Proposition 6.3** (Eq. (8.6) in \([41]\) or \([6]\)). If \( y = \mu + \varepsilon \) with \( \varepsilon \sim N(0, \sigma^2 I_n) \) and \( f : \mathbb{R}^n \to \mathbb{R}^n \) has weakly differentiable components then

\[ \mathbb{E}[(\varepsilon^\top f(y) - \sigma^2 \text{div } f(y))^2] = \sigma^2 \mathbb{E}[\|f(y)\|^2] + \sigma^4 \mathbb{E}[\text{Tr}(\|
abla f(y)\|^2)] \]

(6.1)

\[ \leq \sigma^2 \mathbb{E}[\|f(y)\|^2] + \sigma^4 \mathbb{E}[\|
abla f(y)\|^2_F] \]

(6.2)

\[ \leq \sigma^2 \mathbb{E}[\|f(y)\|^2] + 2\sigma^4 \mathbb{E}[\|
abla f(y)\|^2_F], \]

provided that the last line is finite. If \( \mathbb{E}[f(y)] = 0 \) then

(6.3)

\[ \mathbb{E}[(\varepsilon^\top f(y) - \sigma^2 \text{div } f(y))^2] \leq 2\sigma^4 \mathbb{E}[\|
abla f(y)\|^2_F]. \]

The first equality in (6.1) is the identity studied in \([6]\) and (6.1) follows by the Cauchy-Schwarz inequality. The second inequality is a consequence of the Gaussian Poincaré inequality \([10, \text{Theorem } 3.20]\) applied to each component of \( f \).

The variant (6.5) below may also be useful.

**Proposition 6.4.** Let \( f, \varepsilon, y \) be as in Proposition 6.3. Then there exist random variables \( Z, T, \hat{T} \)

with \( Z \sim N(0, 1) \) and \( \mathbb{E}[\hat{T}^2] \vee \mathbb{E}[T^2] \leq 1 \) such that

(6.4)

\[ |\varepsilon^\top f(y) - \sigma^2 \text{div } f(y)| \leq \sigma |Z| \cdot \|f(y)\| + \sigma^2 2|T| \cdot \mathbb{E}[\|
abla f(y)\|^2_F]^{1/2} \]

(6.5)

\[ \leq \sigma |Z| \cdot \|f(y)\| + \sigma^2 (2|T| + |Z\hat{T}|) \mathbb{E}[\|
abla f(y)\|^2_F]^{1/2}. \]
Proof. Define $F(y) = f(y) - E[f(y)]$, $Z = \sigma^{-1} \varepsilon^T E[f(y)] / \|E[f(y)]\| \sim N(0, 1)$ and

$$T^2 = (\varepsilon^T f(y) - 2\sigma\|E[f(y)]\|)^2 / (2\sigma^4\|\nabla f(y)\|^2)$$

Since $E[F(y)] = 0$, by (6.2) applied to $F$ we have

$$2\sigma^4\|\nabla f(y)\|^2 E[T^2] = E[(\varepsilon^T F(y) - \varepsilon^T F(y))^2] \leq 2\sigma^4 E[\|\nabla f(y)\|^2] = 2\sigma^4 E[\|\nabla f(y)\|^2]$$

so that $E[T^2] \leq 1$. Next, let $\tilde{T} = [\sigma^2 E[\|\nabla f(y)\|^2]^{1/2} \|E[f(y)]\|] - \|f(y)\|$, which satisfies $E[\tilde{T}^2] \leq 1$ by the Gaussian Poincaré inequality. By construction of $T$ and $\tilde{T}$, we obtain (6.5). \qed

**Proposition 6.5.** Let $X = (x_{ij}) \in \mathbb{R}^{n \times p}$ with iid $N(0, 1)$ entries and $\eta : \mathbb{R}^{n \times p} \to \mathbb{R}^p, \rho : \mathbb{R}^{n \times p} \to \mathbb{R}^n$ two vector valued functions, with weakly differentiable components $\eta_1, \ldots, \eta_p$ and $\rho_1, \ldots, \rho_n$. Then

$$E\left[\left(\rho^T X \eta - \sum_{i=1}^n \sum_{j=1}^p \frac{\partial (\rho_i \eta_j)}{\partial x_{ij}}\right)\right] = E\left[\left(\|\rho\|^2 \|\eta\|^2 + \sum_{i=1}^n \sum_{j=1}^p \sum_{k=1}^n \frac{\partial (\rho_i \eta_j)}{\partial x_{ik}} \frac{\partial (\rho_i \eta_k)}{\partial x_{ij}}\right)\right]$$

$$\leq E\left[\|\rho\|^2 \|\eta\|^2 + \sum_{i=1}^n \sum_{j=1}^p \left\|\frac{\partial (\rho_i \eta_j)}{\partial x_{ij}}\right\|^2\right]$$

(6.6)

provided that the second line is finite, where for brevity we write $\rho = \rho(X), \eta = \eta(X)$, and similarly for the partial derivatives (i.e., omitting the dependence in $X$).

**Proof of Proposition 6.5.** Proposition 6.5 is obtained for $X$ with iid $N(0, 1)$ entries by applying (6.1) to $y = \varepsilon = \text{vec}(X)$ and $f(X) = \text{vec}(\rho(X) \eta(X)^T)$ where $\text{vec}(\cdot)$ is the vectorization operator. \qed

## 7. $\chi^2$ Type Bounds Under Dependence

To prove Theorem 7.2 and Corollary 2.5, we first derive a lemma to control the correlation between the two mean-zero random variables

$$\|z_j f(z_k)\|^2 - \|f(z_k)\|^2 \quad \text{and} \quad \|z_k h(z_j)\|^2 - \|h(z_j)\|^2$$

where $z_j, z_k$ are independent standard normal random vectors and $f, h$ are functions $\mathbb{R}^n \to \mathbb{R}^n$. If $f, h$ are constant, then the correlation between these two random variables is 0 by independence. If $f, h$ are non-constant, the following gives an exact formula and an upper bound for the correlation of the two random variables in (7.1).

**Lemma 7.1.** Let $z_j, z_k$ be independent $N(0, I_n)$ random vectors. Let $f, h : \mathbb{R}^n \to \mathbb{R}^n$ deterministic with weakly differentiable components and define the random matrices $A, B \in \mathbb{R}^{n \times n}$ respectively by $A = (z_j^T f(z_k)I_n + f(z_k)z_j^T)\nabla f(z_k)^T$ and $B = (z_k^T h(z_j)I_n + h(z_j)z_k^T)\nabla h(z_j)^T$. Assume that

$$E[\|f(z_k)\|^4] + E[\|h(z_j)\|^4] + E[\|A\|_F^2] + E[\|B\|_F^2] < +\infty.$$

Then equality

$$E[\{(z_j^T f(z_k))^2 - \|f(z_k)\|^2\} \{(z_k^T h(z_j))^2 - \|h(z_j)\|^2\}] = E[\text{Tr}\{AB\}]$$

holds and $E[\text{Tr}[AB]] \leq 4E[\|\nabla f(z_k)\|^2 \|f(z_k)\|^2]^{1/2}E[\|\nabla h(z_j)\|^2 \|h(z_j)\|^2]^{1/2}$. \hfill (7.3)

**Proof.** Define $z \in \mathbb{R}^{2n}$ with $z = (z_j^T, z_k^T)^T$ as well as $F, H : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ by

$$F\left(\begin{bmatrix} z_j \\ z_k \end{bmatrix}\right) = \left(\begin{bmatrix} f(z_k) \\ f(z_k) \end{bmatrix} \begin{bmatrix} z_j \\ z_k \end{bmatrix}\right), \quad H\left(\begin{bmatrix} z_j \\ z_k \end{bmatrix}\right) = \left(\begin{bmatrix} 0_{n \times n} \\ h(z_j)h(z_j)^T \end{bmatrix} \begin{bmatrix} z_j \\ z_k \end{bmatrix}\right).$$

The Jacobians of $F, H$ are the $2n \times 2n$ matrices

$$\nabla F(z)^T = \begin{bmatrix} f(z_k) & A \\ 0_{n \times n} & 0_{n \times n} \end{bmatrix}, \quad \nabla H(z)^T = \begin{bmatrix} 0_{n \times n} & 0_{n \times n} \\ B & h(z_j)h(z_j)^T \end{bmatrix}.$$
Since div $F(z) = \text{Tr}[\nabla F(z)] = \|f(z_k)\|^2$ and similarly for div $H$, the left hand side in (7.3) equals
$$E[(z^\top F(z) - \text{div} F(z))(z^\top H(z) - \text{div} H(z))]$$
with $F, H$ being weakly differentiable with $E[\|F(z)\|^2 + \|H(z)\|^2 + \|\nabla H(z)\|^2] < +\infty$ thanks to (7.2). The last display is equal to $E[\|F(z)^\top H(z) + \text{Tr}(\nabla F(z) H(z))\|$ by Section 2.2 in [6]. Here $F(z)^\top H(z) = 0$ always holds by construction of $F, H$ and the matrix product by block gives $\text{Tr}(\nabla H(z) \nabla F(z)) = \text{Tr}(AB)$.

Next, by the Cauchy-Schwarz inequality we have $E[\text{Tr}(AB)] \leq E[\|A\|_F \|B\|_F] \leq E[\|A\|_F^2]^{1/2} E[\|B\|_F^2]^{1/2}$. By definition of $A$ and properties of the operator norm,
$$\|A\|_F \leq \|\nabla f(z_k)\|_F \|z_j^\top f(z_k)\| + \|f(z_k)\|_F \|\nabla f(z_k)z_j\|.$$
For the non-diagonal terms we compute $\mathbb{E}[\chi_j \chi_k]$ using Lemma 7.1 with $f^{(j,k)}(z_k) = \mathbb{E}_j[\rho]$ and $h^{(j,k)}(z_j) = \mathbb{E}_k[\rho]$ conditionally on $(z_i)_{i \neq (j,k)}$. Thanks to $\|\rho\| \leq 1$ this gives

$$\mathbb{E}[\chi_j \chi_k] \leq C_39 \mathbb{E} \left[ \sum_{i=1}^{n} \left( \left\| \frac{\partial \mathbb{E}_i[\rho]}{\partial x_{ij}} \right\|^2 + \left\| \frac{\partial \mathbb{E}_j[\rho]}{\partial x_{ik}} \right\|^2 \right) \right] \leq C_39 \mathbb{E} \left[ \sum_{i=1}^{n} \left( \left\| \frac{\partial \rho}{\partial x_{ij}} \right\|^2 + \left\| \frac{\partial \rho}{\partial x_{ik}} \right\|^2 \right) \right],$$

where the second inequality follows by dominated convergence for the conditional expectation (i.e., $(\partial/\partial x_{ij}) \mathbb{E}_i[\rho] = \mathbb{E}_k[(\partial/\partial x_{ij}) \rho]$ almost surely) and Jensen’s inequality. Finally, summing over all pairs $j \neq k$ we find

$$\sum_{j=1}^{p} \left( \sum_{k=1}^{p} \mathbb{E}[\chi_j \chi_k] \right) \leq C_39 \mathbb{E} \left[ \left( \sum_{j=1}^{p} \sum_{k=1}^{n} \left\| \frac{\partial \mathbb{E}_j[\rho]}{\partial x_{ij}} \right\|^2 \right) + \left( \sum_{k=1}^{n} \sum_{i=1}^{n} \left\| \frac{\partial \mathbb{E}_j[\rho]}{\partial x_{ik}} \right\|^2 \right) \right] = 2pC_39 \mathbb{E} \sum_{j=1}^{p} \sum_{i=1}^{n} \left\| \frac{\partial \rho}{\partial x_{ij}} \right\|^2.$$

(iv) For the last term, using $\|\mathbb{E}_j[\rho]\|^2 - \|\rho\|^2 \leq \|\mathbb{E}_j[\rho] - \rho\| \|\mathbb{E}_j[\rho] + \rho\|$ and the Cauchy-Schwarz inequality we find

$$\sum_{j=1}^{p} \left( \sum_{k=1}^{p} \mathbb{E}[\chi_j \chi_k] \right) \leq C_39 \mathbb{E} \left[ \left( \sum_{j=1}^{p} \sum_{k=1}^{n} \left\| \frac{\partial \mathbb{E}_j[\rho]}{\partial x_{ij}} \right\|^2 \right) \right] \leq \mathbb{E} \left[ \left( \sum_{j=1}^{p} \sum_{i=1}^{n} \left\| \frac{\partial \rho}{\partial x_{ij}} \right\|^2 \right) \right] \leq \sqrt{4p}.$$

By Lemma 6.1, $\mathbb{E}[\|X\|^2_{op}] \leq (\sqrt{p} + \sqrt{n})^2$. Thus if $\|\rho\| \leq 1$ a.s., the right-hand side of (6.6) is bounded from above by an absolute constant times $RHS^2$ where $RHS$ is defined in Corollary 2.5. By the Cauchy-Schwarz inequality to lower bound the left-hand side of (6.6),

$$\mathbb{E}[\|X^\top \rho\|^2 - p\|\rho\|^2 - \sum_{i=1}^{n} \sum_{j=1}^{p} \left[ e_j^\top X \rho \frac{\partial \rho}{\partial x_{ij}} + \rho_i e_j^\top X \frac{\partial \rho}{\partial x_{ij}} \right] \right] = \mathbb{E}[\|X^\top \rho\|^2 - \sum_{i=1}^{n} \sum_{j=1}^{p} \frac{\partial \rho}{\partial x_{ij}} \rho_{ij}^2] \leq C_{40} RHS.$$

By definition of $RHS$ and expanding the square in (7.4) we also have

$$\mathbb{E}[p \|\rho\|^2 - \|X^\top \rho\|^2 + 2 \sum_{i=1}^{n} \sum_{j=1}^{p} e_j^\top X \rho \frac{\partial \rho}{\partial x_{ij}} - \sum_{j=1}^{p} \left( \sum_{i=1}^{n} \frac{\partial \rho}{\partial x_{ij}} \right)^2 ] \leq C_{41} RHS.$$

If the left-hand sides of the two previous displays are written as $\mathbb{E}[U]$ and $\mathbb{E}[V]$ then the left-hand side of (2.16) is exactly $\mathbb{E}[U + V]$ (cancelling out $\|X^\top \rho\|^2 - p\|\rho\|^2$) and the left-hand side of (2.15) is exactly $\mathbb{E}[2U + V]$ (cancelling out $2 \sum_{i=1}^{n} \sum_{j=1}^{p} e_j^\top X \rho \frac{\partial \rho}{\partial x_{ij}}$).
8. Rotational invariance of regularized least-squares

The crux of the following proposition is the rotational invariance of the design. As in the rest of the paper, let \((X, \varepsilon)\) be independent such that \(X\) has iid \(N(0, \Sigma)\) rows. Consider \(R \in O(n)\) a random rotation distributed according to the Haar measure (i.e., such that \(R u\) is uniformly distributed on the sphere for any deterministic \(u\) with \(\|u\| = 1\)). Then by rotational invariance of the Gaussian measure of \(X\), \((\tilde{X}, \tilde{\varepsilon}) \equiv (RX, R\varepsilon)\) is such that \(\tilde{X}\) has iid \(N(0, \Sigma)\) rows and \(\tilde{\varepsilon}\) is independent of \(X\) with the uniform distribution on the sphere of radius \(\|\varepsilon\|\). If \(\tilde{\beta}\) is a penalized \(M\)-estimator with square loss as in (3.1) then \(\tilde{\beta}(\varepsilon + X\beta, X) = \tilde{\beta}(R\varepsilon + RX\beta, RX)\) because \(\|R(y - Xb)\|^2 = \|y - Xb\|^2\) for all \(b \in \mathbb{R}^p\). Thus the distribution of \(\tilde{\beta}\) is unchanged if the noise \(\varepsilon\) is replaced by \(\tilde{\varepsilon} = \|\varepsilon\|_2 v\) where \(v\) is uniformly distributed on the sphere of radius 1 and independent of \((X, \|\varepsilon\|)\).

**Proposition 8.1.** Set \(p/n = u^2/2\). Let \(\tilde{\beta}\) in (3.1) and \(\hat{df}\) in (2.4). Assume that \(y\) has continuous distribution with respect to the Lebesgue measure. Assume that \(X\) has iid \(N(0, \Sigma)\) rows and that \(\varepsilon\) is independent of \(X\). Then \(E[\xi^2] \leq C_{42}/n\) for

\[
(8.1) \quad \xi = \frac{(y - X\tilde{\beta})^T \varepsilon - \|\varepsilon\|^2(1 - \hat{df}/n)}{(\|\varepsilon\|^4 + \|\varepsilon\|^2\|y - X\tilde{\beta}\|^2)^{1/2}}.
\]

Consequently, the random variable \(\text{Rem}\) defined just before (3.5) satisfies

\[
|\text{Rem}| = (n - \hat{df})\left| \frac{(y - X\tilde{\beta})^T \varepsilon - \|\varepsilon\|^2(1 - \hat{df}/n)}{\|y - X\tilde{\beta}\|^2 + n\|\Sigma^{1/2} h\|^2} \right| = \xi (n - \hat{df})\left| \frac{(\|\varepsilon\|^4 + \|\varepsilon\|^2\|y - X\tilde{\beta}\|^2)^{1/2}}{\|y - X\tilde{\beta}\|^2 + n\|\Sigma^{1/2} h\|^2} \right|
\]

and using \(\|\varepsilon\| \leq \|y - X\tilde{\beta}\| + \|X\Sigma^{-1/2}\|_{\text{op}}\|\Sigma^{1/2} h\|\) to bound the rightmost numerator,

\[
(8.2) \quad E[\text{Rem}] \leq C_{43} n E[\xi^2]^{1/2}(1 + E[\|n^{-1/2}X\Sigma^{-1/2}\|_{\text{op}}^4]^{1/2}) \leq C_{44}(\gamma)\sqrt{n}
\]

if \(p/n \leq \gamma\) by Lemma 6.1.

**Proof of Proposition 8.1.** As explained above the proposition, let \(R \in O(n)\) be a random rotation independent of \((\varepsilon, X)\), so that \((RX, \|\varepsilon\|)\) is independent of \(z \equiv R\varepsilon/\|\varepsilon\|\). Conditionally on \((RX, \|\varepsilon\|)\), define the function \(f : \mathbb{R}^n \to \mathbb{R}^n\) by \(f(z) \equiv z - \|\varepsilon\|\Sigma^{-1} R(R^\top z + X\beta, X) - \beta\) so that \(f(z) = \|\varepsilon\|^{-1}R(y - X\beta)\) and \(\|f(z)\| = \|\varepsilon\|^{-1}\|y - X\beta\|\). Then dividing the numerator and denominator by \(\|\varepsilon\|^2\) in (8.1),

\[
\xi = \frac{f(z)^\top z - (1 - \hat{df}/n)}{\sqrt{1 + \|f(z)\|^2}}.
\]

With \(H = (\partial/\partial y)(X\tilde{\beta}(y, X))\) holding \(X\) fixed, viewing \(y = \|\varepsilon\| R^\top z + X\beta\) as a function of \(z\) we have by the chain rule \(\nabla f(z)^\top = I_n - RR^\top\). Since \(H\) is almost surely positive semi-definite with eigenvalues in \([0, 1]\) by Proposition 2.2, this proves that \(f\) is 1-Lipschitz. By the chain rule, \(\tilde{f}(z) \equiv f(z)/\sqrt{1 + \|f(z)\|^2}\) has Jacobian

\[
(8.3) \quad \nabla \tilde{f}(z)^\top = \frac{\nabla f(z)^\top}{\sqrt{1 + \|f(z)\|^2}} - \frac{f(z) f(z)^\top}{(1 + \|f(z)\|^2)^{3/2}}
\]

which has operator norm bounded by 2, hence \(\tilde{f}(z)\) is 2-Lipschitz. Since \(z\) is uniformly distributed on the sphere, with \(P_z = (I_n - zz^\top)\), \([8, \text{Lemma B.1}]\) shows

\[
E[(n\tilde{f}(z)^\top z - \text{Tr}[\nabla \tilde{f}(z)^\top P_z])] \leq n E[\|\tilde{f}(z)\|^2] + (1 - \frac{2}{n})^{-1} E[\|\nabla \tilde{f}(z)^\top P_z\|^2] = C_{45} n.
\]
Since \( \text{Tr}[\nabla f(z)^\top] = n - \hat{d}f \) and \( |\text{Tr}[\nabla \tilde{f}(z)^\top P_z] - (1 + \|f(z)\|^2)^{1/2}(n - \hat{d}f)| \leq C_{46} \) a.s. by (8.3),
\[
\mathbb{E}(n\xi)^2 = \mathbb{E}[|n\tilde{f}(z)^\top z - (1 + \|f(z)\|^2)^{-1/2}\text{Tr}[\nabla f(z)^\top]|^2]
\leq 2\mathbb{E}[|n\tilde{f}(z)^\top z - \text{Tr}[\nabla \tilde{f}(z)^\top P_z]|^2] + 2\mathbb{E}[|\text{Tr}[\nabla \tilde{f}(z)^\top P_z] - (1 + \|f(z)\|^2)^{-1/2}(n - \hat{d}f)|^2]
\leq C_{47}n + C_{48}.
\]

### 9. Proofs of auxiliary results

#### 9.1. Proof of some properties of the Jacobian \( V = (\partial/\partial y)\hat{\psi} \).

**Proposition 2.2.** Assume that \( \rho \) is convex differentiable and that \( \psi = \rho' \) is 1-Lipschitz. For every fixed \( X \in \mathbb{R}^{n \times p} \) the following holds.

- For almost every \( y \), the map \( y \mapsto \hat{\psi} = \psi(y - X\hat{\beta}) \) is Frechet differentiable at \( y \), and the Jacobian \( V = (\partial/\partial y)\hat{\psi} \in \mathbb{R}^{n \times n} \) is symmetric psd with operator norm at most one so that \( \text{Tr}[V] = \text{Tr}[(\partial/\partial y)\hat{\psi}] \in [0, n] \).

- If additionally Assumption 2.3(i) or (iii.b) holds then almost surely \( \hat{d}f \leq |\hat{I}| \) where \( \hat{I} = \{i \in [n] : \psi'(y_i - x_i^\top\hat{\beta}) > 0\} \) is the set of inliers.

The following lemma is useful to prove Proposition 2.2.

**Lemma 9.1.** Assume that \( \rho \) is convex differentiable and that \( \psi = \rho' \) is 1-Lipschitz. Then \( \rho(u) = \min_{v \in \mathbb{R}} \{ (u - v)^2/2 + h(v) \} \) for some convex function \( h \). Consider

\[
(\hat{b}, \hat{\theta}) \in \arg\min_{b \in \mathbb{R}^p, \theta \in \mathbb{R}^n} \|y - Xb - \theta\|^2/(2n) + g(b) + \sum_{i=1}^n h(\theta_i)/n.
\]

Then for every solution \( \hat{\beta} \) to the optimization problem (1.2), there exists a solution \( (\hat{b}, \hat{\theta}) \) to the optimization problem (9.1) such that \( \hat{\beta} = \hat{b} \) and \( \psi(y - X\hat{\beta}) = y - X\hat{b} - \hat{\theta} \).

**Proof of Proposition 9.1.** If \( \psi = \rho' \) is 1-Lipschitz then \( f(u) = u^2/2 - \rho \) is convex and 1-smooth (in the sense that \( f' \) is again 1-Lipschitz), so that its Fenchel conjugate \( f^*(v) = \max_{u \in \mathbb{R}} \{ uv - f(u) \} \) is 1-strongly convex (in the sense that \( v \mapsto f^*(v) - v^2/2 \) is convex). Let \( h(v) = f^*(v) - v^2/2 \). For this choice of \( h \), we have thanks to \( f^{**} = f \)
\[
\min_{v \in \mathbb{R}} \left\{ \frac{(u - v)^2}{2} + h(v) \right\} = \frac{u^2}{2} - \max_{v \in \mathbb{R}} \{ uv - f^*(v) \} = \frac{u^2}{2} - \left( \frac{u^2}{2} - \rho(u) \right) = \rho(u).
\]
If \( \rho \) is the Huber loss (2.7) this construction was already well studied and in this case \( h(v) = |v| \), see for instance [21, Section 6] or [16] and the references therein.

Next consider the M-estimator with square loss and design matrix \([X|I_n] \in \mathbb{R}^{n \times (p+n)} \) defined by (9.1). The KKTT conditions are given by

\[
X^\top (y - X\hat{b} - \hat{\theta}) \in n\partial g(\hat{b}), \quad y_i - x_i^\top\hat{b} - \hat{\theta}_i \in \partial h(\hat{\theta}_i), \quad i \in [n]
\]

where \( \partial g \) and \( \partial h \) denote the subdifferentials of \( g \) and \( h \). That is, \((\hat{b}, \hat{\theta})\) is solution to (9.1) if and only if (9.2) holds. We claim that one solution of the optimization problem (9.1) is given by \((\hat{b}, \hat{\theta}) = (\hat{\beta}, y - X\hat{\beta} - \psi(y - X\hat{\beta}))\) where \( \hat{\beta} \) is any solution in (1.2). Indeed, the first part in (9.2) holds by the optimality conditions \( X^\top \psi(y - X\hat{\beta}) \in n\partial g(\hat{\beta}) \) of \( \hat{\beta} \) as a solution to the optimization problem (1.2); it remains to check that \( y_i - x_i^\top\hat{b} - \hat{\theta}_i \in \partial h(\hat{\theta}_i) \) holds for all \( i \in [n] \), or equivalently that

\[
\psi(y_i - x_i^\top\hat{\beta}) \in \partial h(y_i - x_i^\top\hat{\beta} - \psi(y_i - x_i^\top\hat{\beta}))
\]
by definition of \( \tilde{\theta} \). By additivity of the subdifferential, \( v + \partial h(v) = \partial f^*(v) \). Furthermore \( u \in \partial f^*(v) \) if and only if \( f^*(u) + f^*(v) = uv \) by property of the Fenchel conjugate, where here we have \( f^*(u) = f(u) = u^2/2 - \rho(u) \) since here \( f \) is convex and finite valued. We also have \( v \in \partial f(u) \) if and only if \( f(u) + f^*(v) = uv \), and hence \( \partial f(u) = \{ u - \psi(u) \} \) is a singleton. Combining these pieces together, for any \( u, v \in \mathbb{R} \) we find

\[
v = u - \psi(u) \quad \text{iff} \quad v \in \partial f(u)
\]

\[
\text{iff} \quad f(u) + f^*(v) = uv
\]

\[
\text{iff} \quad f^*(u) + f^*(v) = uv
\]

\[
\text{iff} \quad u \in \partial f^*(v)
\]

\[
\text{iff} \quad u - v \in \partial h(v).
\]

Hence taking \( u = y_i - x_i^\top \hat{\beta} \) and \( v = u - \psi(u) \), the previous sentence implies that \( \psi(u) \in \partial h(u - \psi(u)) \) and the previous display (9.3) must hold for all \( i \in [n] \). This proves that the given \( (\hat{b}, \hat{\theta}) \) is solution to (9.1).

Proof of Proposition 2.2. By [7, Proposition J.1] applied to \( (\hat{b}, \hat{\theta}) \) with design matrix \( [X|I_n] \), the map \( y \mapsto y - X\hat{b} - \hat{\theta} \) is 1-Lipschitz on \( \mathbb{R}^n \), and for almost every \( y \in \mathbb{R}^n \) this map has symmetric positive semi-definite Jacobian. Since \( y - X\hat{b} - \hat{\theta} = \psi(y - X\hat{\beta}) \), this proves the first bullet point of Proposition 2.2.

For the second bullet point, under Assumption 2.3(iii-a) the claim is proved in Proposition 2.4. Under Assumption 2.3(i) or (ii), by Lemma 2.6 and (2.21) we have \( V = (\partial / \partial y) \hat{\psi} = D(I_n - (\partial / \partial y)X\hat{\beta}) = D(I_n - X\hat{\beta}X^\top D) \) where \( D = \text{diag}(\psi') \). If \( H = (\partial / \partial y)(X\hat{\beta}) = X\hat{\beta}X^\top D \), we bound \( \hat{d}f = \text{Tr} H \) as follows: if \( D^\top \) denotes the pseudo-inverse of \( D \), using the commutation property of the trace and \( D = DD^\top D \),

\[
|\hat{I} - \hat{d}f| = \text{Tr}[D^\top D - H] = \text{Tr}[DD^\top - X\hat{\beta}X^\top D D^\top D] = \text{Tr}[(D^\top)^{1/2}V(D^\top)^{1/2}] \geq 0
\]

where the last inequality is thanks to \( V \) being symmetric psd. This proves \( \hat{d}f \leq |\hat{I}| \).

9.2. Elastic-Net penalty and Huber Lasso.

Proof of Proposition 2.3. The KKT conditions read \( X^\top \hat{\psi} - n\mu \hat{\beta} \in n\lambda \partial \| \hat{\beta} \|_1 \) where \( \partial \| b \|_1 \) denotes the sub-differential of the \( \ell_1 \) norm at \( b \in \mathbb{R}^p \). We first prove that the KKT conditions hold strictly with probability one, in the sense that

\[
P(\forall j \in [p], \ j \notin S \text{ implies } e_j^\top X^\top \hat{\psi} \in (-n\lambda, n\lambda)) = 1.
\]

Let \( j_0 \) be fixed and let \( \tilde{\alpha} \) be the solution to the same optimization problem as \( \hat{\beta} \), with the additional constraint that the \( j_0 \)-th coordinate is always set to 0. Then \( \{ j_0 \notin S \} = \{ \tilde{\alpha} = \hat{\beta} \} \) as the solution of each optimization problem is unique thanks to \( \mu > 0 \). Let \( X_{-j_0} \) be \( X \) with \( j_0 \)-th column removed. The conditional distribution of \( X e_{j_0} \) given \( (X_{-j_0}, y) \) is continuous because \( (X, y) \) has continuous distribution. Hence \( e_{j_0}^\top X^\top \hat{\psi}(y - X\hat{\alpha}) \) also has continuous distribution conditionally on \( (X_{-j_0}, y) \) when \( \hat{\psi}(y - X\hat{\alpha}) \neq 0 \), so that \( P(e_{j_0}^\top X^\top \hat{\psi}(y - X\hat{\alpha}) \in \{-\lambda n, \lambda n\}|X_{-j_0}, y) = 0 \) because a continuous distribution has no atom. The unconditional probability is also 0 by the tower property. This shows that \( P(j_0 \notin S \text{ and } e_{j_0}^\top X^\top \hat{\psi} \in (-n\lambda, n\lambda)) = 0 \) for all \( j_0 \). The union bound over all \( j_0 \in [p] \) proves that the KKT conditions hold strictly with probability one, as desired.

The maps \( (y, X) \mapsto \hat{\beta} \) and \( (y, X) \mapsto \hat{\psi} \) are Lipschitz continuous on every compact by Proposition 4.2(i) as \( \Sigma \) is invertible. At a point \( (y_0, X_0) \) where the KKT conditions hold strictly,
the KKT conditions stay strict and \( \hat{S} \) stay the same in a neighborhood of \((y_0, X_0)\) because the continuity of \((y, X) \mapsto e_j^T X^T \psi - n \mu \beta_j\) ensure that \(e_j^T X^T \psi - n \mu \beta_j\) stay bounded away from \([-n\lambda, n\lambda]\) for every \(j \in [p]\) not in the active set at \((y_0, X_0)\). Furthermore, by (4.2) there exists an open set \(U \subset \mathbb{R}^n \times \mathbb{R}^{n \times p}\) with \(U \ni (y_0, X_0)\) such that the maps \((y, X) \mapsto \hat{\beta}\) and \((y, X) \mapsto \hat{\psi}\) are Lipschitz in \(U\), and the chain rule (2.21) yields \((\partial/\partial y) \hat{\psi} = \text{diag}(\psi')(I_n - X(\partial/\partial y)\hat{\beta})\) for almost every \((y, X) \in U\). In a neighborhood of a point \((y_0, X_0)\) where the KKT conditions hold strictly and where the aforementioned chain rule holds, since \(\hat{S}\) is locally constant we have \((\partial/\partial y) \hat{\beta}_{\hat{S}^c} = 0_{\hat{S}^c \times [n]}\) as well as

\[
X^T \text{diag}(\psi') [I_n - X(\partial/\partial y)\hat{\beta}] - n \mu (\partial/\partial y)\hat{\beta} = 0_{\hat{S}^c \times [n]}.
\]

By simple algebra, this implies \((\partial/\partial y) \hat{\beta}_{\hat{S}^c} = (X^T \text{diag}(\psi') X_{\hat{S}^c} + \mu n I_{|\hat{S}|})^{-1} X^T \text{diag}(\psi')\) and the desired expressions for \((\partial/\partial y) X \hat{\beta}\) and \((\partial/\partial y) \hat{\psi}\).

\[
\]

Proof of Proposition 2.4. For the Huber loss with \(\ell_1\)-penalty, the M-estimator \(\hat{\beta}\) satisfies

\[
(\hat{\beta}, \hat{\theta}) = \arg \min_{(b, \theta) \in \mathbb{R}^p \times \mathbb{R}^n} \|Xb + \kappa \theta - y\|^2 / (2n) + \lambda(\|b\|_1 + \|\theta\|_1)
\]

where \(\kappa > 0\) is some constant, see e.g. [16] and the references therein or Proposition 9.1 with \(h(\cdot)\) proportional to \(|\cdot|\) for the Huber loss. Let \(\bar{\beta} = (\hat{\beta}, \hat{\theta})\). Then \(\bar{\beta}\) is a Lasso solution with data \((y, X)\) where the design matrix is \(X = [X|\kappa I_n] \in \mathbb{R}^{n \times (n+p)}\).

In this paragraph, we show that if \(X\) has continuous distribution then \(X\) satisfies Assumption 3.1 of [6] with probability one. That assumption requires that for any \((\delta_j)_{j \in [p+n]} = \{-1, +1\}^{p+n}\) and any columns \(c_{j_1}, ..., c_{j_{n+1}}\) of \(X\) with \(j_1 < ... < j_{n+1}\), the matrix

\[
\left(\begin{array}{ccc}
  c_{j_1} & \cdots & c_{j_{n+1}} \\
  \delta_{j_1} & \cdots & \delta_{j_{n+1}}
\end{array}\right) \in \mathbb{R}^{(n+1) \times (n+1)}
\]

has rank \(n+1\). We reorder the columns so that any column of the form \(c_{p+i}, i \in [n]\) is the \(i\)-th column after reordering, and note that \(c_{p+i} = \kappa e_i\). Then there exists a value of \(X \in \mathbb{R}^{n \times p}\) such that the above matrix, after reordering the columns, is equal to

\[
\left(\begin{array}{c|c}
  \kappa I_n & 0_{n \times 1} \\
  \delta_{k_1} & \cdots & \delta_{k_n} & \delta_{k_{n+1}}
\end{array}\right)
\]

for some permutation \((k_1, ..., k_{n+1})\) of \((j_1, ..., j_{n+1})\). Since the previous display has nonzero determinant \(\kappa^n \delta_{k_{n+1}}\), the determinant of matrix (9.4), viewed as a polynomial of the coefficients of \(X\), is a non-zero polynomial. Since non-zero polynomials have a zero-set of Lebesgue measure 0 [28], this proves that (9.4) is rank \(n+1\) with probability one.

Hence with probability one, by Proposition 3.9 in [6], the solution \(\bar{\beta} \in \mathbb{R}^{n+p}\) is unique, \(\|\bar{\beta}\|_0 \leq n\) and the KKT conditions of the optimization problem of \(\bar{\beta}\) hold strictly almost everywhere in \((y, X)\) (see [45] for related results). This shows that the sets \(\hat{S}\) and \(\hat{I}\), viewed as a function of \(y\) while \(X\) is fixed, are constant in a neighborhood of \(y\) for almost every \((y, X)\). Now the set of \(i \in [n] : \hat{\theta}_i \neq 0\) exactly correspond to the outliers \(i \in [n] : \psi'(y_i - x_i^T \hat{\beta}) = 0\) = \([n] \setminus \hat{I}\) and \(\|\bar{\beta}\|_0 \leq n\) holds if and only if \(|\hat{S}| + (n - |\hat{I}|) \leq n\). This proves that \(|\hat{S}| \leq |\hat{I}|\) almost surely. Furthermore, almost surely in \((y, X)\), the derivative of \(y \mapsto X \bar{\beta} = X \hat{\beta} + \kappa \hat{\theta}\) exists and is equal to the orthogonal projection onto the linear span of \(\{e_i, i \in [n] \setminus \hat{I}\} \cup \{X e_j, j \in \hat{S}\}\). We construct an orthonormal basis of this linear span as follows: First by considering the vectors \(\{e_i, i \in [n] \setminus \hat{I}\}\) and then completing by a basis \((u_k)_{k \in \hat{S}}\) of the orthogonal complement of \(\{e_i, i \in [n] \setminus \hat{I}\}\). Note that this orthogonal complement is exactly the column span of \(\text{diag}(\psi') X_{\hat{S}}\). The orthogonal projection onto the linear span of
\{e_i, i \in [n] \setminus \hat{I}\} \cup \{X e_j, j \in \hat{S}\} is thus (\partial/\partial y)X \hat{\beta} = \sum_{i \in [n] \setminus \hat{I}} e_i e_i^T + \sum_{k \in \hat{S}} u_k u_k^T. Since \text{diag}(\psi') is constant in a neighborhood of \(y\) and \text{diag}(\psi') zeros out all rows corresponding to outliers,
\[
\text{diag}(\psi')(\partial/\partial y)X \hat{\beta} = (\partial/\partial y)\text{diag}(\psi')X \hat{\beta} = (\partial/\partial y)\text{diag}(\psi')X \hat{\beta} = \text{diag}(\psi')(\partial/\partial y)X \hat{\beta} = \sum_{k \in \hat{S}} u_k u_k^T
\]
which is exactly the orthogonal projection \(\hat{Q}\) defined in the proposition, as desired. The almost sure identity \((\partial/\partial y)\hat{\psi} = \text{diag}(\psi') - \hat{Q}\) is obtained by the chain rule: Here \(\psi\) is differentiable at \(y_i - x_i^T \hat{\beta}\) for all \(i \in [n]\) with probability one since the fact that the KKT conditions of \(\hat{\beta}\) hold strictly imply that no \(y_i - x_i^T \hat{\beta}\) is a kink of \(\psi\).

10. LASSO: LIPSCHITZ CONDITIONS

Lemma 10.1 (deterministic argument). Let \(n, \bar{p} \geq 1\) be integers and \(m \in [\bar{p}]. Let \(A \in \mathbb{R}^{n \times \bar{p}}, and define the Lasso \(\hat{b} = \arg \min_{b \in \mathbb{R}^{\bar{p}}} \|Ab - \overline{y}\|^2 / (2n) + \frac{1}{\sqrt{n}} \|b\|_1\) where \(\overline{y} = Ab^* + z\) for some \(b^* \in \mathbb{R}^{\bar{p}}. Then
\[
\|\hat{b}\|_0 \leq \phi_{\max}(A^T A) \max \left\{ \frac{2\|z\|^2}{\lambda^2 n}, \frac{4\|b^*\|_0}{n\kappa^2} \right\} \text{ where } \kappa^2 = \inf_{b \in \mathbb{R}^{\bar{p}}: \|b\|_1 < \|b^*\|_1} \left[ \frac{\|A(b - b^*)\|^2}{n\|b - b^*\|^2} \right].
\]

Let \(\hat{A} \in \mathbb{R}^{n \times \bar{p}} and \(\hat{b} = \arg \min_{b \in \mathbb{R}^{\bar{p}}} \|\hat{A}b - (\hat{A}b^* + z)\|^2 / (2n) + \frac{1}{\sqrt{n}} \|b\|_1\). Then for any \(\text{psd } \Sigma \in \mathbb{R}^{\bar{p} \times \bar{p}},
\[
\min \left\{ 1, \|\hat{A}(\hat{b} - b^*)\|^2 / \|\Sigma^{1/2}(\hat{b} - b^*)\|^2 \right\} \max \left\{ \|\Sigma^{1/2}(\hat{b} - b^*)\|, \|\hat{A}\hat{b} - A\hat{b}\| \right\} \leq \left[ \|\hat{A} - A\|\Sigma^{-1/2}\|_{\text{op}} \right] \|\overline{y} - A\hat{b}\| + \left[ \|\Sigma^{1/2}(\hat{b} - b^*)\| \right](1 + 2\|A\Sigma^{-1/2}\|_{\text{op}})
\]
Proof. The KKT conditions read \(A^T(\overline{y} - X \hat{b}) = \lambda \sqrt{n} \hat{\psi} \|\hat{b}\|_1\). Multiplying the KKT conditions by \(\hat{b} - b^*\) we obtain
\[
\|A(\hat{b} - b^*)\|^2 + \|\hat{A}\hat{b} - \overline{y}\|^2 \leq \|z\|^2 + 2\sqrt{n}\lambda(\|b^*\|_1 - \|\hat{b}\|_1).
\]
We distinguish two cases, based on which of the two terms in the right-hand side is greater. If \(\|z\|^2 \geq 2\sqrt{n}\lambda(\|b^*\|_1 - \|\hat{b}\|_1)\) then we find \(\|A\hat{b} - \overline{y}\|^2 \leq 2\|z\|^2\), and using the KKT conditions gives \(\|\hat{b}\|_0 \leq \frac{1}{\sqrt{n}} \|A^T(\overline{y} - A\hat{b})\|^2 \leq \phi_{\max}(A^T A)2\|z\|^2 / (\lambda^2 n)\). Otherwise, we have \(\|z\|^2 < 2\sqrt{n}\lambda(\|b^*\|_1 - \|\hat{b}\|_1)\) and
\[
\|A(\hat{b} - b^*)\|^2 + \|\hat{A}\hat{b} - \overline{y}\|^2 < 4\sqrt{n}\lambda(\|b^*\|_1 - \|\hat{b}\|_1) \leq 4\sqrt{n}\lambda\|b^*\|_0^{1/2}\|b^* - \hat{b}\| \leq 4\lambda\|b^*\|_0^{1/2}\kappa^{-1}\|A(\hat{b} - b^*)\|.
\]
Using \(4uv \leq 4u^2 + v^2\) for \(v = \|A(\hat{b} - b^*)\|\), the term \(v^2\) cancel out and \(\|\overline{y} - A\hat{b}\|^2 \leq 4\lambda^2\|b^*\|_0\kappa^{-2}\). Using again \(\lambda^2 n\|\hat{b}\|_0 \leq \|A^T(\overline{y} - A\hat{b})\|^2 \leq \phi_{\max}(A^T A)\|\overline{y} - A\hat{b}\|^2\) completes the proof of (10.1). By the same argument as the proof of Proposition 4.5 with \(\mu_p = 1\) (square loss) we obtain (10.2).
depending on \((d_*, \gamma, \varphi, a_*)\) only such that as \(n, p \to +\infty\) while \((d_*, \gamma, \varphi, a_*)\) remain fixed we have
\[
\tag{10.3}
\Pr(\forall h \in \mathbb{R}^p : \|\Sigma^{1/2}h\| = 1, \|h\|_0 \leq d_* n \Rightarrow \|\frac{1}{\sqrt{n}}Xh\| > t_1) \to 1,
\]
\[
\tag{10.4}
\Pr(\forall h \in \mathbb{R}^p : \|\Sigma^{1/2}h\| = 1, \|h\|_1 \leq 2\sqrt{k_2 n}\|h\|_2 \Rightarrow \|\frac{1}{\sqrt{n}}Xh\| > t_2) \to 1,
\]
\[
\tag{10.5}
\Pr(\forall h, \theta \in \mathbb{R}^{p+n} : \|\Sigma^{1/2}h\|^2 + \|\theta\|^2 = 1, \|h\|_0 + \|\theta\|_0 \leq d_* n \Rightarrow \|\frac{1}{\sqrt{n}}Xh + a_\theta\| > t_3) \to 1,
\]
\[
\tag{10.6}
\Pr(\forall h, \theta \in \mathbb{R}^{p+n} : \|\Sigma^{1/2}h\|^2 + \|\theta\|^2 = 1, \|h\|_1 + \|\theta\|_1 = 1 \Rightarrow \|\frac{1}{\sqrt{n}}Xh + a_\theta\| > t_4) \to 1.
\]

In the following proof, for a random matrix \(Z \in \mathbb{R}^{n \times p}\) and two subspaces \(V_L \subset \mathbb{R}^n\) and \(V_R \subset \mathbb{R}^p\) of dimension \(d_L\) and \(d_R\) respectively, we call the restriction of \(Z\) to \(V_L\) and \(V_R\) the random matrix \(G = Q_L^TZQ_R \in \mathbb{R}^{d_L \times d_R}\) where \(Q_L \in \mathbb{R}^{n \times d_L}\), \(Q_R \in \mathbb{R}^{p \times d_R}\) have orthonormal columns such that \(Q_LQ_L^T\) is the orthogonal projection onto \(V_L\) and \(Q_RQ_R^T\) is the orthogonal projection onto \(V_R\). If \(Z\) has iid \(N(0, 1)\) entries then \(G\) also has iid \(N(0, 1)\) entries by rotational invariance.

**Proof.** The proof of (10.3) is a minor variant of the union bound argument in [9, Proposition 2.10]. In short, thanks to the explicit formula for the smallest density of a Wishart matrix with identity covariance from [24], the argument in [15, Proof of Lemma 4.1] gives \(\Pr(\phi_{\min}(G^T G/n) \leq t^2) \leq \left(\frac{et}{n-d+\pi}e^{-et}\right)^{n-d-1} / \sqrt{2\pi(n-d+1)}\) if \(G \in \mathbb{R}^{n \times d}\) has iid \(N(0, 1)\) entries. With \(d = \min\{d_L, d_R\}\), we apply this inequality to all \((\frac{p}{d})\) Gaussian matrices obtained as the restriction of \(X \Sigma^{-1/2}\) to a \(d\)-dimensional subspace generated as the span of \(d\) columns of \(\Sigma^{1/2}\). Taking the union bound, the probability of the union is bounded from above by \((\frac{p}{d})\left(\frac{et}{n-d+\pi}\right)^{n-p-1} / \sqrt{2\pi(n-d+1)}\) which converges to 0 if \(t\) is a small enough constant thanks to \((\frac{p}{d})\leq e^{d\log(e/d)}\). By a direct application of [32, Lemma 2.7], (10.4) is then obtained by choosing the constant \(k_2 = k_2(d_*, \gamma, \varphi) > 0\) small enough.

Next we focus on (10.5). We do not attempt to optimize the constants. The event \(|X \Sigma^{-1/2}|_{op} \leq 2\sqrt{n} + \sqrt{p}\) has probability approaching one [17, Theorem II.13]. In this event, simultaneously for all \((h, \theta)\) such that \(a_{\pi} \|\theta\| \geq \max\{a_{\pi}, (2 + \sqrt{\gamma})\}\|\Sigma^{1/2}h\|\), the triangle inequality
\[
\|\frac{1}{\sqrt{n}}Xh + a_\theta\| \geq a_\theta\|\theta\| - (2 + \sqrt{\gamma})\|\Sigma^{1/2}h\| \geq a_{\pi}\|\theta\| \quad \text{thanks to } a_{\pi}\|\theta\| \geq (2 + \sqrt{\gamma})\|\Sigma^{1/2}h\|
\]
\[
\geq a_{\pi}\|\Sigma^{1/2}h\| + \|\theta\| \quad \text{thanks to } \|\Sigma^{1/2}h\|^2 \leq \|\theta\|^2.
\]
We now consider \((h, \theta)\) such that the reverse inequality \(a_{\pi}\|\theta\| < \max\{a_{\pi}, (2 + \sqrt{\gamma})\}\|\Sigma^{1/2}h\|\) holds. Let \(O \subset [n]\) and \(S \subset [p]\) be such that \(|O| + |S| = \min\{d_L, d_R\}\) and let \(G \in \mathbb{R}^{(n-|O|) \times |S|}\) be the Gaussian matrix obtained by restriction of the Gaussian matrix \(X \Sigma^{-1/2}\) restricted on the left to the rows indexed in \([n]\)\(\setminus O\), and on the right to the subspace given by the linear span of \(\{\Sigma^{1/2}e_j, j \in S\}\). For any \(\theta\) supported in \(O\) and \(h\) supported in \(S\), since the orthogonal projection \(P_O^+ = \sum_{i \in [n] \setminus O} e_i e_i^T\) decreases the norm,
\[
\|\frac{1}{\sqrt{n}}Xh + a_\sqrt{n}\theta\| \geq \|\frac{1}{\sqrt{n}}P_O^+Xh\| = \|\frac{1}{\sqrt{n}}G\Sigma^{1/2}h\| \geq a_{\pi}\|\Sigma^{1/2}h\| \geq \phi_{\min}(G^T G/n)\|\Sigma^{1/2}h\|.
\]
We again resort to the union bound argument in [9, Proposition 2.10] to control \(\phi_{\min}(G^T G/n)\). As in the proof of (10.3) for a Gaussian matrix with \(n - |O|\) rows and \(|S|\) columns we have [15, Proof of Lemma 4.1]
\[
\Pr(\phi_{\min}(G^T G/n) \leq t^2) \leq \left(\frac{et}{n-|O|-|S|+1}\right)^n \left(\frac{en}{|O|-|S|+1}\right)^{|S|} \leq \left(\frac{et}{(1-d_*)+1}\right)^{n(1-d_*)+1} / \sqrt{2\pi(n-|O|-|S|+1)}
\]
thanks to \(n - |O| - |S| \geq n(1 - d_*)\) and the fact that \(u \mapsto \frac{1}{\sqrt{u}}\) is decreasing on \([1/e, +\infty)\). There are \(\binom{n+p}{d_*, n}\) possible pairs \((O, S)\) with \(|O| + |S| = \min\{d_L, d_R\}\). Using \(\binom{N}{d} \leq \exp[d \log(eN/d)]\) for
integers \( d \leq N \), a union bound leads to an extra multiplicative factor at most \( \exp(nd \log(e^{1/2})) \) in the previous display. Choosing \( t > 0 \) a small enough constant depending on \((\gamma, d_*)\) only, the probability of the union over all pairs \((S, O)\) with \(|S| + |O| = |d_* n|\) of such events over converge to 0. This completes the proof of (10.5) to obtain \( r_3 > 0 \) depending only on \((d_*, \gamma, \gamma_*)\). Finally, (10.6) is again obtained from (10.5) and [32, Lemma 2.7] by choosing the constant \( k_4 \in (0, 1) \) small enough and depending only on \((t_3, \varphi, d_*, \gamma, \gamma_*)\).

\[ \square \]

**Proposition 10.3.** Let \( d_* \in (0, 1), \varphi > 1, \gamma > 1 \) be arbitrary constants. Assume \( p/n \leq \gamma \) and let \( X \) have iid rows with distribution \( N(0, \Sigma) \) with \( \Sigma_{jj} = 1 \) for all \( j \in [p] \) and \( \|\Sigma\|_{op} \leq \varphi \). Assume that the noise \( \varepsilon \) has iid \( N(0,1) \) entries. Then there exist constants \( s_*,\lambda_* \) depending only on \((d_*, \varphi, \gamma)\) such that if \( \|\beta\|_0 \leq s_* n \) and \( \beta = \arg \min_{\beta \in \mathbb{R}^p} \|X \beta - y\|^2/(2n) + \lambda n^{-1/2} \|\beta\|_1 \) with \( \lambda \geq \sigma \lambda_* \), there exists an open set \( \Omega_L \subset \mathbb{R}^n \times \mathbb{R}^{n \times p} \) such that \( (\varepsilon, X) \in \Omega_L \Rightarrow \|\hat{\beta}\|_0 \leq d_* n/2 \) and \( \mathbb{P}(\varepsilon, X) \in \Omega_L) \rightarrow 1 \) as \( n, p \rightarrow +\infty \) while \((d_*, \varphi, \gamma)\) remain fixed. Furthermore, with \( \varepsilon, \tilde{\varepsilon} \in \mathbb{R}^n \) with \( \varepsilon = \tilde{\varepsilon}, \tilde{X}, X \in \mathbb{R}^{n \times p} \) and \( \beta, \tilde{\beta}, \psi, \tilde{\psi}, \tilde{r}, r \) the corresponding quantities as in Lemma 4.3, then \( \{(\varepsilon, X), (\varepsilon, \tilde{X})\} \subset \Omega_L \) implies

\[
(10.7) \quad \left( \frac{1}{n} \|\psi - \tilde{\psi}\|^2 + \|\Sigma \frac{1}{n} (\tilde{\beta} - \beta)\|^2 \right)^{1/2} \leq n^{-1/2} L_* \left( \|X - \tilde{X}\| \Sigma^{-1/2} \|\psi\|^2 + \|\Sigma \frac{1}{n} (\tilde{\beta} - \beta)\|^2 \right)^{1/2}
\]

for a constant \( L_* = L_*(d_*, \gamma, \varphi) > 0 \) depending only on \((d_*, \gamma, \varphi)\).

**Proof.** Let \( t_1, t_2, k_2 \) be the constants in (10.4) and note that \( t_1, t_2, k_2 \) depend only on \((d_*, \gamma, \varphi)\). Define \( s_* = s_*(d_*, \gamma, \varphi) \), \( \lambda_* = \lambda_*(d_*, \gamma, \varphi) > 0 \) and \( \Omega_L \subset \mathbb{R}^n \times \mathbb{R}^{n \times p} \) by

\[
(10.8) \quad s_* = \min \left\{ k_2, \frac{d_* t_2^2}{8 \varphi^2 (2 + \sqrt{\gamma})^2} \right\}, \quad \lambda_* \equiv \frac{\varphi (2 + \sqrt{\gamma})^2}{d_*},
\]

\[ \Omega_L = \{ (\varepsilon, X) : \|\varepsilon\| < \sigma \sqrt{1.01n}; X \text{ satisfies the events in (10.3), (10.4): } \|X \Sigma^{-1/2}\|_{op} < \sqrt{n} (2 + \sqrt{\gamma}) \} \]

Thanks to (10.1) with \( A = X, \ z = \varepsilon \) and \( p = \tilde{p} \) we have in \( \Omega_L \)

\[
\|\beta\|_0 \leq s_* n \Rightarrow \|\beta\|_0 \leq k_2 n \Rightarrow \left( \frac{1}{\kappa^2} \leq \frac{\varphi}{t_2^2} \right) \quad \text{and} \quad \|\tilde{\beta}\|_0 \leq \varphi n (2 + \sqrt{\gamma}) \max \left\{ \frac{2.02 \sigma^2}{\lambda^2}, \frac{4 \|\beta\|_{op}}{nt_2^2} \right\}
\]

where \( \kappa^2 \) is defined in (10.1). Above, the bound \( \frac{1}{\kappa^2} \leq \frac{\varphi}{t_2^2} \) follows from the definition of \( \kappa, t_2 \) and

\[
\left( \|\beta\|_1 - \|\tilde{\beta}\|_1 \right) + \|\tilde{\beta} - \beta\|_1 \leq 2 \sum_{j \in S} |\tilde{\beta}_j - \beta_j| \leq 2 \|\beta\|_0^{1/2} \left( \sum_{j \in S} (\tilde{\beta}_j - \beta_j)^2 \right)^{1/2} \leq 2 \|\beta\|_0^{1/2} \|\tilde{\beta} - \beta\|_2.
\]

By construction of \( s_*, \lambda_* \) in (10.8), \( \|\beta\|_0 \leq s_* n \) and \( \lambda \geq \sigma \lambda_* \) implies that in the event \( \Omega_L \), the upper bound on \( \|\tilde{\beta}\|_0 \) is smaller than \( d_* n/2 \) so that \( \|\tilde{\beta}\|_0 \leq d_* n/2 \) holds.

The fact that \( \mathbb{P}(\varepsilon, X) \in \Omega_L) \rightarrow 1 \) from a standard bound on the deviation of the \( \chi^2 \) random variable \( \|\varepsilon\|^2/\sigma^2 \), (10.3)-(10.4) and Lemma 6.1.

To prove (10.7), if \( (\varepsilon, X), (\varepsilon, \tilde{X}) \in \Omega_L \) then \( \|\tilde{\beta} - \beta\|_0 \leq d_* n \) so that \( \|X (\tilde{\beta} - \beta)\| > \sqrt{n} t_1 \|\Sigma^{1/2} (\tilde{\beta} - \beta)\| \) by (10.3). Applying the last part of Lemma 10.1 to \( A = X, \tilde{A} = \tilde{X}, \ z = \varepsilon, \Sigma = n \Sigma \) and \( b = \beta, \tilde{b} = \tilde{\beta} \) we obtain \( \|A (b - \tilde{b})\| \geq t_1 \sqrt{n} \|\Sigma^{1/2} (b - \tilde{b})\| = t_1 \|\Sigma^{1/2} (b - \tilde{b})\| \) to bound from below the minimum in the left-hand side of (10.2) which gives (10.7).

\[ \square \]

**Proof of Theorem 2.1 and Theorem 3.1 for the Lasso, under Assumption 2.3(iii.a).** Let \( d_* \in (0,1) \) be any absolute constant in \((0,1)\), e.g., \( d_* = 0.99 \). We make explicit the change of variable to create a new isotopic design matrix: Let

\[
(10.9) \quad G \equiv X \Sigma^{-1/2}, \quad w = \Sigma^{1/2} (\beta - \beta)
\]
so that $G$ has iid $N(0,1)$ entries. Let $L_*$ and $\Omega_L$ be given by Proposition 10.3. For $U = \{ G \in \mathbb{R}^{n \times p} : (\varepsilon, G\Sigma^{-1/2}) \in \Omega_L \}$ and $\psi, \rho : \mathbb{R}^{n \times p} \rightarrow \mathbb{R}, D : \mathbb{R}^{n \times p} \rightarrow \mathbb{R}$ the functions defined by

\begin{equation}
(10.10) \quad \psi(G) = \psi(y - X\hat{\beta}) = \psi(\varepsilon - Gw), \quad D(G) = (\|\varepsilon\|^2/n + \|w\|^2)^{1/2}, \quad \rho(G) = n^{-1/2}\psi(G)/D(G)
\end{equation}

we have $\|\rho(G) - \rho(G')\| \leq 2L_*n^{-1/2}\|G - G'\|_F$ by (4.6) if $\{G, G'\} \subset U$. Applying Corollary 2.7 conditionally on $\varepsilon$ to $\rho(G)$, to the random matrix $G$ and to $L = 2L_*$, (2.34) gives that

\begin{equation}
(10.11) \quad \text{Rem}_L \overset{\text{def}}{=} \|G^\top\rho\|^2 - p\|\rho\|^2 - \sum_{k=1}^p \sum_{i=1}^n \frac{\partial \rho_i}{\partial g_{ij}}^2 - 2\sum_{i=1}^n \sum_{k=1}^p \rho_i e_k G^\top \frac{\partial \rho}{\partial g_{ij}}
\end{equation}

has $E[I(\Omega)\text{Rem}_L] \leq C_{49}(\gamma, d_*, \varphi)\sqrt{n}$ where $\Omega$ is the event $\Omega = \{(\varepsilon, G\Sigma^{1/2}) \in \Omega_L\}$. The derivatives of $y - X\hat{\beta}$ with respect to $X$ and for a fixed $\varepsilon$ are given by [7, Proposition 4.1]: for almost every $(\varepsilon, X)$, Frechet differentiability holds at $X$ and the derivatives are given (holding $\varepsilon$ fixed) by

\begin{equation}
\frac{\partial}{\partial \varepsilon_{ij}} (y - X\hat{\beta}) = -X \hat{\Delta} e_j(y_i - x_i^\top \hat{\beta}) - V e_i(\hat{\beta}_j - \beta_j).
\end{equation}

where $\hat{S} = \{j \in [p] : \hat{\beta}_j \neq 0\}$, $X_S \in \mathbb{R}^{n \times |\hat{S}|}$ is the submatrix of $X$ made of the columns of $X$ indexed in $\hat{S}$, and

\begin{equation}
(10.12) \quad \hat{A}_{\hat{S},\hat{S}} = (X^\top_S X_S)^{-1} \text{ and } \hat{A}_{jk} = 0 \text{ if } j \notin \hat{S} \text{ or } k \notin \hat{S}, \quad V = I_n - X\hat{\Delta}X^\top.
\end{equation}

Consequently, by the chain rule using $X = G\Sigma^{1/2}$, the derivatives of $\psi(G)$ are given by

\begin{equation}
(10.13) \quad \frac{\partial}{\partial g_{ij}} \psi(G) = -GAe_k \psi_i - V e_i w_k \quad \text{ where } \quad A = \Sigma^{1/2}\hat{\Delta} \Sigma^{1/2} \in \mathbb{R}^{p \times p}
\end{equation}

and where $w = (w_k)_{k=1,...,p}$ is the vector in (10.9). At this point, the argument and algebra are the same as those of (2.27) and (2.30); using the same argument as in the discussion surrounding (2.27)-(2.30) we find with $d\!f = \text{Tr}[GAG^\top] = \text{Tr}[X\hat{\Delta}X^\top] = |\hat{S}|$ that almost surely

\begin{equation}
(10.14) \quad \left| 2\sum_{k=1}^p \sum_{i=1}^n \rho_i e_k G^\top \frac{\partial \rho}{\partial g_{ij}} + 2d\!f\|\rho\|^2 \right| \leq 2\|Gn^{-1/2}\|_{op} + 2L_*\|Gn^{-1/2}\|_{op},
\end{equation}

In $\Omega$, thanks to (10.3) and $\|\hat{\beta}\|_0 \leq d_* n/2$ to bound from above $\|\hat{\Sigma}\|_{op}$ and thanks to $\|X\Sigma^{-1/2}\|_{op} \leq \sqrt{n}(2 + \sqrt{7})$ in the event $\Omega_L$ in (10.8), the right-hand sides of the two displayed equations above are bounded from above by $C_{50}(\gamma, \varphi, d_*)$. Multiplying by $I(\Omega)$ and taking expectation gives

\begin{equation}
\begin{aligned}
E[I(\Omega)\|G^\top\rho\|^2 - (p - 2d\!f)\|\rho\|^2 - \text{Tr}[V]^2\|w\|^2/(nD^2)] &\leq C_{51}(\gamma, \varphi, d_*) + E[I(\Omega)\text{Rem}_L] \\
&\leq C_{52}(\gamma, \varphi, d_*) \sqrt{n}.
\end{aligned}
\end{equation}

Since $\|\hat{\beta}\|_0 \leq d_* n/2$ in $\Omega$, the proof of Theorem 2.1 under Assumption 2.3(iii.a) for the Lasso is complete. The proof of Theorem 3.1 follows a similar adaptation of the proof given in Section 3, using (2.35) applied to $\rho(G)$, $G$ and $L = 2L_*$ on the one hand and Proposition 8.1 on the other. \hfill \Box

11. HUBER LASSO: LIPSCHITZ CONDITIONS

This section provides the necessary lemmas to prove the main result under Assumption 2.3(iii.a) and (iii.b). Assumption (iii.b) corresponds to the $\ell_1$ penalty combined with a scaled Huber loss is used as the loss function: for tuning parameters $\lambda_H, \lambda$,

\begin{equation}
\hat{\beta} = \arg \min_{b \in \mathbb{R}^p} \left( \frac{1}{n} \sum_{i=1}^n \lambda_H^2 \rho_H \left( \lambda_H^{-1}(y_i - x_i^\top b) \right) + n^{-1/2} \lambda \|b\|_1 \right)
\end{equation}
where $\rho_H$ is the Huber loss (2.7). We let $\hat{O} = \{ i \in [n] : \psi'(y_i - x_i^T \hat{\beta}) = 0 \}$ be the set of outliers.

To control the sparsity and number of outliers of the M-estimator with Huber loss and $\ell_1$ penalty (11.1), the following equivalent definition of the estimator will be useful. The M-estimator $\hat{\beta} \in \mathbb{R}^p$ is equal to the first $p$ components of the solution $(\hat{\beta}, \hat{\theta}) \in \mathbb{R}^{p+n}$ of the optimization problem

$$
(11.2) \quad (\hat{\beta}, \hat{\theta}) = \arg \min_{(\beta, \theta) \in \mathbb{R}^{p+n}} \|Xb + \sqrt{n}/(\lambda_H)\theta - y\|^2/(2n) + n^{-1/2}\lambda(\|\theta_1\|_1 + \|\beta\|_1).
$$

This representation of the Huber Lasso $\hat{\beta}$ is well known in the study of M-estimators based on the Huber loss, cf. [21, Section 6] or [16] and the references therein. Since (11.2) reduces to a Lasso optimization problem in $\mathbb{R}^{p+n}$ with design matrix $[X|\sqrt{n}/(\lambda_H)I_n] \in \mathbb{R}^{n \times (p+n)}$ and response $\tilde{y}$, any Lasso solver can be used to compute the robust penalized estimator $\hat{\beta}$ and we can use Lemma 10.1 to control $\|\hat{\beta}\|_0 + \|\hat{\beta}\|_0$. Note that $a_\ast = \frac{\lambda}{\lambda_H}$ under Assumption 2.3(iii.b) so that the design matrix is (11.2) is $[X|\sqrt{n}/(\lambda_H)I_n] \in \mathbb{R}^{n \times (p+n)}$.

Assumption 2.3(iii.b) requires that $(\epsilon_1)_{i \in [n]} \backslash O$ are iid $N(0, \sigma^2)$. As in [16], rewrite $\tilde{y}$ as

$$(11.3) \quad \tilde{y} = X\beta^* + \sqrt{n}/a_\ast \theta^* + z \quad \text{where} \quad z_i = 0 \quad \text{for} \quad i \in O \quad \text{and} \quad (z_i)_{i \in [n] \backslash O} = (\epsilon_i)_{i \in [n] \backslash O} \sim \text{iid} N(0, \sigma^2)$$

where $\theta^*$ is supported on $O \subset [n]$ with $\|\theta^*\|_0 \leq |s_n| - \|\beta\|_0$. The non-zero components of the unknown vector $\theta^*$ represent the contaminated responses and $\theta^*$ is not independent of $z$. The sparsity of the unknown regression vector in the above linear model with design matrix $\bar{X} = [X|\sqrt{n}/a_\ast I_n]$ is $\|\beta\|_0 + \|\theta^*\|_0 \leq s_n$, and the support of $\hat{\theta}$ is exactly the set of outliers $\hat{O} = \{ i \in [n] : \psi'(y_i - x_i^T \hat{\beta}) = 0 \}$. Lemma 10.1 shows that $\|\hat{\beta}\|_0 + \|\hat{\theta}\|_0$ can be controlled with high probability when $s_\ast \in (0, 1)$ is a small enough constant and the tuning parameter is large enough, and (10.5)-(10.6) are used to control the $\kappa$ constant in (10.1).

**Proposition 11.1.** Let $d_\ast \in (0, 1), \varphi > 1, \gamma > 1, a_\ast > 0$ be arbitrary constants. Assume $p/n \leq \gamma$ and let $X$ have iid entries with distribution $N(0, \Sigma)$ with $\Sigma_{jj} = 1$ for all $j \in [p]$ and $\|\Sigma\|_{op} \|\Sigma^{-1}\|_{op} \leq \varphi$. Assume that the noise $\varepsilon$ has iid $N(0, 1)$ entries. Then there exist constants $s_\ast, \lambda_\ast$ depending only on $(d_\ast, \varphi, \gamma, a_\ast)$ such that if $\|\beta\|_0 + \|\theta^*\|_0 \leq s_n$, and $(\hat{\beta}, \hat{\theta})$ is the minimizer of (11.2) with $\lambda/\lambda_H = a_\ast$ and $\lambda \geq \sigma\lambda_\ast$, there exists an open set $\Omega_H \subset \mathbb{R}^n \times \mathbb{R}^{n \times p}$ such that $(\varepsilon, X) \in \Omega_H \Rightarrow \|\hat{\beta}\|_0 + \|\hat{\theta}\|_0 \leq d_n/2$ and $\mathbb{P}((\varepsilon, X) \in \Omega_H) \rightarrow 1$ as $n, p \rightarrow +\infty$ while $(d_\ast, \varphi, \gamma, a_\ast)$ remain fixed. Furthermore, with $\varepsilon, \hat{\varepsilon} \in \mathbb{R}^n$ with $\varepsilon = \hat{\varepsilon}$, $\bar{X}, \tilde{X} \in \mathbb{R}^{n \times p}$, and $\hat{\beta}, \hat{\theta}, \hat{\psi}, \hat{\psi}, \hat{\theta}, \hat{\tilde{X}}$ the corresponding quantities as in Lemma 4.3, then $\{(\varepsilon, X), (\varepsilon, \tilde{X})\} \subset \Omega_H$ implies (10.7) for a constant $L_\ast = L_\ast(d_\ast, \varphi, \gamma, a_\ast) > 0$ depending only on $(d_\ast, \varphi, \gamma, a_\ast)$.

**Proof.** We need to specify constants $s_\ast \in (0, 1)$ and $\lambda_\ast > 0$. Let $O \subset [n]$ be as in (11.3). Define

$\Omega_H = \{ (\varepsilon, X) : \varepsilon_{[n] \backslash O} < \sqrt{1.01} \sqrt{n}; \; X \; \text{satisfies the events in} \; (10.5), (10.6); \; \|X\Sigma^{-1/2}\|_{op} < \sqrt{n}(2 + \sqrt{\gamma}) \}.$

Let $t_3, t_4, k_4$ be the constants in (10.5)-(10.6). Thanks to (10.1) with $A = [X|\sqrt{n}a_\ast I_n] \in \mathbb{R}^{n \times (p+n)}$, $z = \varepsilon$ and $p = n + m$ we have in $\Omega_H$

$$
\|\beta\|_0 + \|\theta^*\|_0 \leq k_4n \quad \Rightarrow \quad \|\hat{\beta}\|_0 + \|\hat{\theta}\|_0 \leq \varphi^2(a_\ast + 2 + \sqrt{\gamma})^2 \max\{\frac{2\varphi^2}{\lambda^2}, \frac{4(\|\beta\|_0 + \|\theta^*\|_0)}{n^2t_4} \}.
$$

As in the proof of Proposition 10.3, we can thus choose $s_\ast(\varphi, t_2, \gamma, d_\ast, a_\ast)$ small enough and $\lambda_\ast = \lambda_\ast(\varphi, t_2, \gamma, d_\ast, a_\ast)$ large enough such that $\|\beta\|_0 + \|\theta^*\|_0 \leq s_n$, $\lambda \geq \sigma\lambda_\ast$ implies that in the event $\Omega_H$, the right-hand side of the previous display is smaller than $d_n/2$, i.e., we have $\|\hat{\beta}\|_0 + \|\hat{\theta}\|_0 \leq d_n/2$. If $(\varepsilon, X), (\varepsilon, \tilde{X}) \in \Omega_H$ then $\|\beta - \beta\|_0 + \|\theta - \theta\|_0 \leq d_n$. Applying Lemma 10.1 to $A = [X|\sqrt{n}a_\ast I_n], \tilde{A} = [\tilde{X}|\sqrt{n}a_\ast I_n], z$ defined in (11.3), $\Sigma \in \mathbb{R}^{(p+n) \times (p+n)}$ diagonal by block with the two blocks $(\Sigma, I_n)$, and $\tilde{b} = [\beta^T | \tilde{\theta}^T], \tilde{\beta} = [\beta^T | \tilde{\theta}^T]$ we obtain $\|A(\tilde{b} - \tilde{b})\| \geq t_3 \sqrt{n}/(\Sigma^{1/2}(\tilde{b} - \tilde{b})^2) + (\|\theta - \theta\|_2^2)^{1/2} = t_3\|\Sigma^{1/2}(\tilde{b} - \tilde{b})\|$ to bound from below the minimum in the left-hand side of (10.2) which gives (10.7). □
Proof of Theorem 2.1 for the Huber Lasso, under Assumption 2.3(iii.b). Let \( d_* \in (0,1) \) be any absolute constant in \((0,1)\), e.g., \( d_* = 0.99 \). Define \( G \in \mathbb{R}^{n \times p} \) and \( w \) by (10.9). Let \( L_* \) and \( \Omega_H \) be given by Proposition 11.1. For \( U = \{ G \in \mathbb{R}^{n \times p} : (\varepsilon, G \Sigma^{-1/2}) \in \Omega_H \} \) and \( \psi, \rho : \mathbb{R}^{n \times p} \to \mathbb{R} \) the functions defined by (10.10), we have \( \| \rho(G) - \rho(G') \| \leq 2 L_* n^{-1/2} \| G - G' \|_F \) by (4.6) if \( \{ G, G' \} \subset U \). Applying Corollary 2.7 conditionally on \( \varepsilon \) to \( \rho(G) \), to the random matrix \( G \) and to \( L = 2 L_* \), (2.34) gives that (10.11) has \( \mathbb{E}|I\{ \Omega \} \text{Rem}_L| \leq C_{5a}(\gamma, d_*, \varphi) \sqrt{n} \) where \( \Omega \) is the event \( \Omega = \{(\varepsilon, G \Sigma^{1/2}) \in \Omega_H \} \).

Using the argument discussed after (9.4) that the KKT conditions of the Huber Lasso hold strictly and some algebra (we omit the details), the derivatives of \( \psi(y - X\hat{\beta}) \) with respect to \( X \) and for a fixed \( \varepsilon \) are given by
\[
\frac{\partial}{\partial x_{ij}} \psi(y - X\hat{\beta}) = -DX\hat{A}e_j \psi(y_i - x_i^T \hat{\beta}) - Ve_i (\hat{\beta}_j - \beta_j).
\]
where \( D = \text{diag}(\psi') \in \mathbb{R}^{n \times n} \), \( \hat{S} = \{ j \in [p] : \hat{\beta}_j \neq 0 \} \), \( X_{\hat{S}} \in \mathbb{R}^{n \times |\hat{S}|} \) is the submatrix of \( X \) made of the columns of \( X \) indexed in \( \hat{S} \), and
\[
(11.4) \quad \hat{A}_{\hat{S}, \hat{S}} = (X_{\hat{S}}^T DX_{\hat{S}})^{-1} \text{ and } \hat{A}_{jk} = 0 \text{ if } j \notin \hat{S} \text{ or } k \notin \hat{S}, \quad V = D - DX\hat{A}X^T D.
\]
Consequently, by the chain rule using \( X = G \Sigma^{1/2} \), the derivatives of \( \psi(G) \) in (10.10) are given almost surely by
\[
(11.5) \quad \frac{\partial}{\partial g_{ik}} \psi(G) = -DG_{ik} e_k \psi_i - Ve_i w_k \quad \text{where} \quad A = \Sigma^{1/2} \hat{A} \Sigma^{1/2} \in \mathbb{R}^{p \times p}
\]
and where \( w = (w_k)_{k=1, \ldots, p} \) is the vector in (10.9). At this point, the argument and algebra are the same as those of (2.27) and (2.30); using the same argument as in the discussion surrounding (2.27)-(2.30) we find with \( df = \text{Tr}[GAG^T D] = \text{Tr}[X\hat{A}X^T D] = |\hat{S}| \) (see Proposition 2.4) that almost surely (10.14) hold. In \( \Omega \), thanks to (10.5) and \( \| \hat{\beta} \|_0 + \| \theta \|_0 \leq d_* n/2 \) to bound from above \( \| \hat{A} \|_{op} \) and thanks to \( \| X \Sigma^{-1/2} \|_{op} \leq \sqrt{m} (2 + \sqrt{\gamma}) \) in the event \( \Omega_H \), the right-hand sides of (10.14) are bounded from above by \( C_{5a}(\gamma, \varphi, d_*) \). Multiplying by \( I\{ \Omega \} \) and taking expectation gives again (10.15) and the proof of Theorem 2.1 under Assumption 2.3(iii.b) is complete. \( \square \)
\begin{align*}
\psi_H'(u) &= 1 \quad [0, 1] \quad 1 \quad 0 \\
\psi_H(u) &= u \quad [1, 1] \quad 1 \\
\rho_H(u) &= \frac{u^2}{2} \quad [1, 0] \quad u - \frac{1}{2}
\end{align*}

\begin{align*}
\psi_0'(u) &= 1 \quad [0, 1] \quad 1 \quad 2 - u \quad 0 \\
\psi_0(u) &= u \quad [1, 2] \quad \frac{1}{2} + 2u - \frac{u^2}{2} \quad \frac{3}{2} \\
\rho_0(u) &= \frac{u^2}{2} \quad [2, 2] \quad \frac{1}{6} - \frac{u}{2} + u^2 - \frac{u^3}{6} - \frac{7}{6} + \frac{3u}{2}
\end{align*}

Table 2. Huber loss \( \rho_H(u) \) and its derivatives, as well as its smoothed version \( \rho_0(u) \) and its derivatives. In the plots, the loss \( \rho \) is shown in brown, \( \psi = \rho' \) in red and \( \psi' \) in blue.

\begin{align*}
\psi_1'(u) &= 1 \quad [0, 1] \quad 1 \quad 2x^3 - 9x^2 + 12x - 4 \quad 0 \\
\psi_1(u) &= u \quad [1, 2] \quad \frac{3}{2} + \frac{(x-2)^3x}{2} \quad \frac{3}{2} \\
\rho_1(u) &= \frac{u^2}{2} \quad [2, 2] \quad \frac{3u^4}{10} - \frac{3x^4}{4} + 2x^3 - 2x^2 + \frac{3x}{2} - \frac{7}{50} \quad \frac{37}{20} + \frac{3(u-2)}{2}
\end{align*}

Table 3. Smooth robust loss \( \rho_1(u) \) and its derivatives for \( u \geq 0 \).

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