Several new methods have been recently proposed for performing valid inference after model selection. An older method is sampling splitting: use part of the data for model selection and the rest for inference. In this paper we revisit sample splitting combined with the bootstrap (or the Normal approximation). We show that this leads to a simple, assumption-free approach to inference and we establish results on the accuracy of the method. In fact, we find new bounds on the accuracy of the bootstrap and the Normal approximation for general nonlinear parameters with increasing dimension which we then use to assess the accuracy of regression inference. We define new parameters that measure variable importance and that can be inferred with greater accuracy than the usual regression coefficients. Finally, we elucidate an inference-prediction trade-off: splitting increases the accuracy and robustness of inference but can decrease the accuracy of the predictions.

“Investigators who use [regression] are not paying adequate attention to the connection - if any - between the models and the phenomena they are studying. ... By the time the models are deployed, the scientific position is nearly hopeless. Reliance on models in such cases is Panglossian ...”

—David Freedman

1 Introduction

We consider the problem of carrying out assumption-free statistical inference after model selection for high-dimensional linear regression. This is now a large topic and a variety of approaches have been considered under different settings – an overview of a subset of these can be found in Dezeure et al. (2015). We defer a detailed discussion of the literature and list of references until Section 1.1.

In this paper, we will use linear models but we do not assume that the true regression function is linear. We show the following:

1. Inference based on sample splitting followed by the bootstrap (or Normal approximation) gives assumption-free, robust confidence intervals under very weak assumptions. No other known method gives the same inferential guarantees.

2. The usual regression parameters are not the best choice of parameter to estimate in the weak assumption case. We propose new parameters, called LOCO (Leave-Out-COvariates) parameters, that are interpretable, general and can be estimated accurately.

3. There is a trade-off between prediction accuracy and inferential accuracy.
4. We provide new bounds on the accuracy of the Normal approximation and the bootstrap to the distribution of the projection parameter (the best linear predictor) when the dimension increases and the model is wrong. We need these bounds since we will use Normal approximations or the bootstrap after choosing the model. In fact, we provide new general bounds on Normal approximations for nonlinear parameters with increasing dimension. This gives new insights on the accuracy of inference in high-dimensional situations. In particular, the accuracy of the Normal approximation for the standard regression parameters is very poor while the approximation is very good for LOCO parameters.

5. The accuracy of the bootstrap can be improved by using an alternative version that we call the image bootstrap. However, this version is computationally expensive. The image bootstrap is discussed in the appendix.

6. We show that the law of the projection parameter cannot be consistently estimated without sample splitting.

We want to emphasize that we do not claim that the LOCO parameter is optimal in any sense. We just aim to show that there exist alternatives to the usual parameters that, when the linear model is not true, (i) are more interpretable and (ii) can be inferred more accurately.

**Problem Setup and Four (Random) Parameters that Measure Variable Importance**

We consider a distribution-free regression framework, where the random pair \( Z = (X, Y) \in \mathbb{R}^d \times \mathbb{R} \) of \( d \)-dimensional covariates and response variable has an unknown distribution \( P \) belonging to a large non-parametric class \( Q_n \) of probability distributions on \( \mathbb{R}^{d+1} \). We make no assumptions on the regression function \( x \in \mathbb{R}^d \mapsto \mu(x) = E\left[Y | X = x\right] \) describing the relationship between the vector of covariates and the expected value of the response variable. In particular, we do not require it to be linear.

We observe \( D_n = (Z_1, \ldots, Z_n) \), an i.i.d. sample of size \( n \) from some \( P \in Q_n \), where \( Z_i = (X_i, Y_i) \), for \( i = 1, \ldots, n \). We apply to the data a procedure \( w_n \), which returns both a subset of the coordinates and an estimator of the regression function over the selected coordinates. Formally,

\[
D_n \mapsto w_n(D_n) = \left( \hat{S}, \hat{\mu}_{\hat{S}} \right),
\]

where \( \hat{S} \), the selected model, is a random, nonempty subset of \( \{1, \ldots, d\} \) and \( \hat{\mu}_{\hat{S}} \) is an estimator of the regression function \( x \in \mathbb{R}^d \mapsto E\left[Y | X_{\hat{S}} = x_{\hat{S}}\right] \) restricted to the selected covariates \( \hat{S} \), where for \( x \in \mathbb{R}^d \), \( x_{\hat{S}} = (x_j, j \in \hat{S}) \) and \( (X, Y) \sim P \), independent of \( D_n \).

The model selection and estimation steps comprising the procedure \( w_n \) need not be related to each other, and can each be accomplished by any appropriate method. The only assumption we impose on \( w_n \) is that the size of the selected model be under our control; that is, \( 0 < |\hat{S}| \leq k \), for a pre-defined positive integer \( k \leq d \) where \( k \) and \( d \) can both increase with sample size. For example, \( \hat{S} \) may be defined as the set of \( k \) covariates with the highest linear correlations with the response
and $\hat{\mu}_{\hat{S}}$ may be any non-parametric estimator of the regression function over the coordinates in $\hat{S}$ with bounded range. Although our framework allows for arbitrary estimators of the regression function, we will be focusing on linear estimators: $\hat{\mu}_{\hat{S}}(x) = \hat{\beta}_{\hat{S}}^\top x_{\hat{S}}$, where $\hat{\beta}_{\hat{S}}$ is any estimator of the of the linear regression coefficients for the selected variables – such as ordinary least squares on the variables in $\hat{S}$. In particular, $\hat{\beta}_{\hat{S}}$ may arise from fitting a sparse linear model, such as the lasso or stepwise-forward regression, in which case estimation of the regression parameters and model selection can be accomplished simultaneously with one procedure.

It is important to emphasize that, since we impose minimal assumptions on the class $Q_n$ of data generating distribution and allow for arbitrary model selection and estimation procedures $w_n$, we will not assume anything about the quality of the output returned by the procedure $w_n$. In particular, the selected model $\hat{S}$ needs not be a good approximation of any optimal model, however optimality may be defined. Similarly, $\hat{\mu}_{\hat{S}}$ may not be a consistent estimator of the regression function restricted to $\hat{S}$. Instead, our concern is to provide statistical guarantees for various criteria of significance for the selected model $\hat{S}$, uniformly over the choice of $w_n$ and over all the distributions $P \in Q_n$.

We will accomplish this goal by producing confidence sets for four random parameters in $\mathbb{R}^{\hat{S}}$, each providing a different assessment of the level of statistical significance of the variables in $\hat{S}$ from a purely predictive standpoint. All of the random parameters under consideration are functions of the data generating distribution $P$, of the sample $D_n$ and, therefore, of its size $n$ and, importantly, of the model selection and estimation procedure $w_n$. Below, $(X, Y)$ denotes a draw from $P$, independent of the sample $D_n$. Thus the distribution of $(X, Y)$ is the same as their conditional distribution given $D_n$.

- **The projection parameter** $\beta_{\hat{S}}$. The linear projection parameter $\beta_{\hat{S}}$ is defined to be the vector of coefficients of the best linear predictor of $Y$ using $X_{\hat{S}}$:

$$\beta_{\hat{S}} = \arg\min_{\beta \in \mathbb{R}^{\hat{S}}} \mathbb{E}_{X,Y} \left[ (Y - \beta^\top X_{\hat{S}})^2 \right],$$

where $\mathbb{E}_{(X,Y)}$ denote the expectation with respect to the distribution of $(X, Y)$. The terminology projection parameters refers to the fact that $X^\top \beta_{\hat{S}}$ is the projection of $Y$ into the linear space of all random variables that can be obtained as linear functions of $X_{\hat{S}}$. For a through discussion and an analysis of the properties of such parameters see Buja et al. (2015). More generally, this type of quantities are also studied in Lee et al. (2016); Taylor et al. (2014); Berk et al. (2013); Wasserman (2014). Note that the projection parameter is well-defined even though the true regression function $\mu$ is not linear. Indeed, it is immediate that

$$\beta_{\hat{S}} = \Sigma_{\hat{S}}^{-1} \alpha_{\hat{S}}$$

(1)

where $\alpha_{\hat{S}} = (\alpha_{\hat{S}}(j) : j \in \hat{S})$, $\alpha_{\hat{S}}(j) = \mathbb{E}[Y X_{\hat{S}}(j)]$ and $\Sigma_{\hat{S}} = \mathbb{E}[X_{\hat{S}} X_{\hat{S}}^\top]$. We remark that the regression projection parameter depends only on the selected model $\hat{S}$, and not any estimate $\hat{\mu}_{\hat{S}}$ of the regression function on the coordinates in $\hat{S}$ that may be implemented in $w_n$.

- **The LOCO parameters** $\gamma_{\hat{S}}$ and $\phi_{\hat{S}}$. Often, statisticians are interested in $\beta_{\hat{S}}$ as a measure of the importance of the selected covariates. But, of course, there are other ways to measure variable importance. We now define two such parameters, which we refer to as *Leave Out
COvariate Inference – or LOCO – parameters, which were originally defined in Lei et al. (2016) and are similar to the variable importance measures used in random forests. The first LOCO parameter is

\[ \gamma_{\hat{S}}(j) = \mathbb{E}_{X,Y} \left[ \left| Y - \hat{\beta}_{\hat{S}(j)}^{\top} X_{\hat{S}(j)} \right| - \left| Y - \hat{\beta}_{\hat{S}}^{\top} X_{\hat{S}} \right| \right] ; \]

(2)

In the above expression, \( \hat{\beta}_{\hat{S}} \) is any estimator of the projection parameter \( \beta_{\hat{S}} \) and \( \hat{\beta}_{\hat{S}(j)} \) and \( \hat{\beta}_{\hat{S}} \) are obtained by re-running the model selection and estimation procedure after removing the \( j \)-th covariate from the data \( D_n \). To be clear, for each \( j \in wS \), \( \hat{S}(j) \) is a subset of size \( k \) of \( \{1, \ldots, d\} \setminus \{j\} \). Notice that the selected model can be different when covariate \( X_j \) is held out from the data, so that the intersection between \( \hat{S}(j) \) and \( \hat{S} \) can be quite smaller than \( k - 1 \). The interpretation of \( \gamma_{\hat{S}}(j) \) is simple: it is the increase in prediction error by not having access to \( X_j \) (in both the model selection and estimation steps). Of course, it is possible to extend the definition of this parameter by leaving out several variables from \( \hat{S} \) at once without additional conceptual difficulties.

The parameter \( \gamma_{\hat{S}} \) has several advantages over the projection parameter \( \beta_{\hat{S}} \): it is more interpretable since it refers directly to prediction error and we shall see that the accuracy of the Normal approximation and the bootstrap is much higher. Indeed, we believe that the widespread focus on \( \beta_{\hat{S}} \) is mainly due to the fact that statisticians are used to thinking in terms of cases where the linear model is assumed to be correct.

The second type of LOCO parameters that we consider are the median LOCO parameters \( \phi_{\hat{S}} = (\phi_{\hat{S}}(j) : j \in \hat{S}) \) with

\[ \phi_{\hat{S}}(j) = \text{median} \left[ \left| Y - \hat{\beta}_{\hat{S}(j)}^{\top} X_{\hat{S}(j)} \right| - \left| Y - \hat{\beta}_{\hat{S}}^{\top} X_{\hat{S}} \right| \right] , \]

(3)

where the median is over the conditional distribution of \((X,Y)\) given \( D_n \). Though one may simply regard \( \phi_{\hat{S}} \) as a robust version of \( \gamma_{\hat{S}} \), we find that inference for \( \phi_{\hat{S}} \) will remain valid under weaker assumptions that the ones needed for \( \gamma_{\hat{S}} \). Of course, as with \( \gamma_{\hat{S}} \), we may leave out multiple covariate at the same time.

• The prediction parameter \( \rho_{\hat{S}} \). It is also of interest to obtain an omnibus parameter that measures how well the selected model will predict future observations. To this end, we define the future predictive error as

\[ \rho_{\hat{S}} = \mathbb{E}_{X,Y} \left[ \left| Y - \hat{\beta}_{\hat{S}}^{\top} X_{\hat{S}} \right| \right] , \]

(4)

where \( \hat{\beta}_{\hat{S}} \) is any estimator the projection parameters \( \beta_{\hat{S}} \).

Remarks.

1. The LOCO and prediction parameters do not require linear estimators. For example we can define

\[ \gamma_{\hat{S}}(j) = \mathbb{E}_{X,Y} \left[ \left| Y - \hat{\mu}_{\hat{S}(j)}(X_{\hat{S}(j)}) \right| - \left| Y - \hat{\mu}_{\hat{S}}(X_{\hat{S}}) \right| \right] , \quad j \in \hat{S}, \]
where \( \hat{\mu}_S \) is any regression estimator restricted to the coordinates in \( \hat{S} \) and \( \hat{\mu}_{S(j)} \) is the estimator obtained after performing a new model selection process and then refitting without covariate \( j \in \hat{S} \). Similarly, we could have

\[
\rho_S = E_{X,Y} \left[ |Y - \hat{\mu}_S(X_S)| \right],
\]

for an arbitrary estimator \( \hat{\mu}_S \). For simplicity, we will focus on linear estimators, although our results about the LOCO and prediction parameters hold even in this more general setting.

2. It is worth reiterating that the projection and LOCO parameters are only defined over the coordinates in \( \hat{S} \), the set of variables that are chosen in the model selection phase. If a variable is not selected then the corresponding parameter is set to be identically zero and is not the target of any inference.

There is another version of the projection parameter defined as follows. For the moment, suppose that \( d < n \) and that there is no model selection. Let \( \beta_n = (X^\top X)^{-1} X^\top \mu_n \) where \( X \) is the \( n \times d \) design matrix, whose columns are the \( n \) vector of covariates \( X_1, \ldots, X_n \), and \( \mu_n = (\mu_n(1), \ldots, \mu_n(n))^\top \), with \( \mu_n(i) = E[Y_i|X_1, \ldots, X_n] \). This is just the conditional mean of the least squares estimator given \( X_1, \ldots, X_n \). We call this the conditional projection parameter. The meaning of this parameter when the linear model is false is not clear. It is a data dependent parameter, even in the absence of model selection. Buja et al. (2015) have devoted a whole paper to this issue. Quoting from their paper:

When fitted models are approximations, conditioning on the regressor is no longer permitted ... Two effects occur: (1) parameters become dependent on the regressor distribution; (2) the sampling variability of the parameter estimates no longer derives from the conditional distribution of the response alone. Additional sampling variability arises when the nonlinearity conspires with the randomness of the regressors to generate a \( 1/\sqrt{n} \) contribution to the standard errors.

Moreover, it is not possible to estimate the distribution of the conditional projection parameter estimate in the distribution free framework. To see that, note that the least squares estimator can be written as \( \hat{\beta}(j) = \sum_{i=1}^n w_i Y_i \) for weights \( w_i \) that depend on the design matrix. Then \( \sqrt{n}(\hat{\beta}(j) - \beta(j)) = \sum_{i=1}^n w_i \epsilon_i \) where \( \epsilon_i = Y_i - \mu_n(i) \). Thus, for each \( j \in \{1, \ldots, d\} \) we have that \( \sqrt{n}(\hat{\beta}(j) - \beta(j)) \) is approximately \( \approx N(0, \tau^2) \), where \( \tau^2 = \sum_i w_i^2 \sigma_i^2 \), with \( \sigma_i^2 = \text{Var}(\epsilon_i|X_1, \ldots, X_n) \). The problem is that there is no consistent estimator of \( \tau^2 \) under the nonparametric models we are considering. Even if we assume that \( \sigma_i^2 \) is constant (an assumption we avoid in this paper), we still have that \( \tau^2 = \sigma^2 \sum_i w_i^2 \) which cannot be consistently estimated without assuming that the linear model is correct. Again, we refer the reader to Buja et al. (2015) for more discussion. In contrast, the projection parameter \( \beta = \Sigma^{-1} \alpha \) is a fixed functional of the data generating distribution \( P \) and is estimable. For these reasons, we focus in this paper on the projection parameter rather than the conditional projection parameter.
Goals and Assumptions

Our main goal is to provide statistical guarantees for each of the four random parameters of variable significance introduced above, under our distribution free framework. For notational convenience, in this section we let \( \theta_S \) be any of the parameters of interest: \( \beta_S, \gamma_S, \phi_S \) or \( \rho_S \).

We will rely on sample splitting: assuming for notational convenience that the sample size is \( 2n \), we randomly split the data \( D_{2n} \) into two halves, \( D_{1,n} \) and \( D_{2,n} \). Next, we run the model selection and estimation procedure \( w_n \) on \( D_{1,n} \), obtaining both \( \widehat{S} \) and \( \widehat{\mu}_S \) (as remarked above, if we are concerned with the projection parameters, then we will only need \( \widehat{S} \)). We then use the second half of the sample \( D_{2,n} \) to construct an estimator \( \widehat{\theta}_S \) and a confidence hyper-rectangle \( \widehat{C}_S \) for \( \theta_S \) satisfying the following properties:

Concentration:
\[
\limsup_{n \to \infty} \sup_{w_n \in W_n} \sup_{P \in Q_n} P(||\widehat{\theta}_S - \theta_S||_\infty > r_n) \to 0 \quad (5)
\]

Coverage validity (honesty):
\[
\liminf_{n \to \infty} \inf_{w_n \in W_n} \inf_{P \in Q_n} P(\theta_S \in \widehat{C}_S) \geq 1 - \alpha \quad (6)
\]

Accuracy:
\[
\limsup_{n \to \infty} \sup_{w_n \in W_n} \sup_{P \in Q_n} P(\nu(\widehat{C}_S) > \epsilon_n) \to 0 \quad (7)
\]

where \( \alpha \in (0, 1) \) is a pre-specified level of significance, \( W_n \) is the set of all the model selection and estimation procedures on samples of size \( n \), \( r_n \) and \( \epsilon_n \) both vanish as \( n \to \infty \) and \( \nu \) is the size of the set (length of the sides of the rectangle) where we recall that \( k = |S| \) is non-random. The probability statements above take into account both the randomness in the sample \( D_n \) and the randomness associated to splitting it into halves.

Remark. The property that the coverage of \( \widehat{C}_S \) is guaranteed uniformly over the entire class \( Q_n \) is known as (asymptotic) honesty (Li, 1989). Note that the confidence intervals are for random parameters (based on half the data) but the uniform coverage, accuracy and concentration guarantees hold marginally.

The statistical guarantees listed above assure that both \( \widehat{\theta}_S \) and \( \widehat{C}_S \) are robust with respect to the choice of \( w_n \). We seek validity over all model selection and estimation rules because, in realistic data analysis, the procedure \( w_n \) can be very complex. In particular, the choice of model can involve: plotting, outlier removal, transformations, choosing among various competing models, etc.. Thus, unless we have validity over all \( w_n \), there will be room for unconscious biases to enter. Note that sample splitting is key in yielding uniform coverage and robustness.

The confidence sets we construct will be hyper-rectangles. The reason for such choice is two-fold. First, once we have a rectangular confidence set for a vector parameter, we immediately have simultaneous confidence intervals for the components of the vector. Secondly, recent results on high dimensional normal approximation of normalized sums by Chernozhukov et al. (2013, 2014) have shown that central limit theorems for hyper-rectangles have only a logarithmic dependence on the dimension.
Depending on the target parameter, the class $Q_n$ of data generating distributions on $\mathbb{R}^{d+1}$ for the pair $(X, Y)$ will be different. We will provide details on each such case separately. However, it is worth noting that inference for the projection parameters calls for a far more restricted class of distributions than the other parameters. In particular, we find it necessary to impose uniform bounds on the largest and smallest eigenvalues of the covariance matrices of all $k$ marginals of the $d$ covariates, as well as bounds on the higher moments of $X$ and on the mixed moments of $X$ and $Y$. We will further assume, in most cases, that the distribution of the pair $(X, Y)$ in $[-A, A]^{d+1}$, for some fixed $A > 0$. Such compactness assumptions are stronger than necessary but allow us to keep the statement of the results and their proofs simpler. In particular, they may be replaced with appropriate tail or moment bounds and not much will change in our analysis and results.

Although we have formulated the guarantees of honest validity, accuracy and concentration in asymptotic terms, all of our results are in fact obtained as finite sample bounds. This allow us to derive consistency rates in $n$ with all the relevant quantities, such as the dimension $d$, the size of the selected model $k$, and the variance and eigenvalue bounds needed for the projection parameters accounted for in the constants (with the exception of $A$, which we keep fixed). As a result, our results remain valid and are in fact most interesting when all these quantities are allowed to change with $n$.

### 1.1 Related Work

The problem of inference after model selection has received much attention lately. Much of the work falls broadly into three categories: inference uniformly over selection procedure, inference with regard to a particular debiased or desparsified model, and inference conditional on model selection. A summary of some of the various methods is in Table 1. We discuss these approaches in more detail in Section 4.

The uniform approach includes POSI (Berk et al., 2013), which constructs valid inferential procedures regardless of the model selection procedure by maximizing over all possible model selections. This method assumes Normality and a fixed, known variance, as well as being computationally expensive. The idea is built upon by later work (Bachoc et al., 2014, 2016), which extend the ideas to other parameters of interest and which allow for heteroskedasticity, non-normality, and model misspecification.

Most other approaches focus on a particular model selection procedure and conduct inference for selections made by that procedure. This includes the literature on debiased or desparsified regularized models, for example Buhlmann (2013), Zhang and Zhang (2014), Javanmard and Montanari (2014), Buhlmann and van de Geer (2015), Dezeure et al. (2016), Zhang and Cheng (2017), van de Geer et al. (2014), Nickl and van de Geer (2013). This work constructs confidence intervals for parameters in high dimensional regression. These can be used for the selected model if a Bonferroni correction is applied. However, these methods tend to assume that the linear model is correct as well as a number of other assumptions on the design matrix and the distribution of errors.

A separate literature on selective inference has focused on inference with respect to the selected model, conditional on the event of that model’s selection. This began with Lockhart et al. (2014),
| Method          | Parameter | Assumptions       | Accuracy                  | Computation | Robust |
|----------------|-----------|-------------------|---------------------------|-------------|--------|
| Debiasing      | True $\beta$ | Very Strong      | $1/\sqrt{n}$              | Easy        | No     |
| Conditional    | Projection | Strong            | Not known                 | Easy        | No     |
| Uniform        | Projection | Strong            | $\sqrt{k/n}$              | NP hard     | Yes    |
| Sample Splitting | Projection | Weak              | $\sqrt{k^5/2 \log k \log n/n}$ | Easy        | Yes    |
| Sample Splitting | LOCO      | None              | $\sqrt{\log(kn)/n}$       | Easy        | Yes    |

Table 1: Different inferential methods. ‘accuracy’ refers to the size of sides of the confidence set. ‘robust’ refers to robustness to model assumptions. The term ‘Very Strong’ means that the linear model is assumed to be correct and that there are incoherence assumptions on the design matrix. ‘Strong’ means constant variance and Normality are assumed. ‘Weak’ means only iid and invertible covariance matrix (for the selected variables). ‘None’ means only iid or iid plus a moment assumption.

but was developed more fully in Lee et al. (2016), Fithian et al. (2014), and Taylor et al. (2014). Further works in this area include Tibshirani et al. (2015), Xiaoying Tian (2015), Loftus and Taylor (2015), Markovic and Taylor (2016), Tibshirani et al. (2016), Markovic et al. (2017). In the simplest version, the distribution of $\sqrt{n}(\hat{\beta}(j) - \beta(j))$ conditional on the selected model has a truncated Gaussian distribution, if the errors are Normal and the covariates are fixed. The cdf of the truncated Gaussian is used as a pivot to get tests and confidence intervals. This approach requires Normality, and a fixed, known variance. While the approach has broadened in later work, the methods still tend to assume fixed design and a known, parametric structure to the outcome.

There have been several additional approaches to this problem that don’t fall in any of these broad categories. While this is a larger literature than can be addressed completely here, it includes early work on model selection Hurvich and Tsai (1990) and model averaging interpretations Hjort and Claeskens (2003); the impossibility results of Leeb and Pötscher (2008), Buja et al. (2015) on random $X$ and model misspecification; methods based on resampling or sample splitting (Chatterjee and Lahiri, 2011, 2013; Efron, 2014; Wasserman and Roeder, 2009; Meinshausen et al., 2009); stability selection (Meinshausen and Bühlmann, 2010; Shah and Samworth, 2013); the conformal inference approach of Lei et al. (2016); goodness-of-fit tests of Shah and Bühlmann (2018); moment-constraint-based uniform confidence sets (Andrews and Guggenberger, 2009); Meinshausen (2015) on inference about groups of variables under general designs; Belloni et al. (2011) in the instrumental variable setting; Belloni et al. (2015) on post-selection inference for $Z$-estimators, and the knockoffs approach of Barber et al. (2015) and later Candes et al. (2016). Although they are not directed at linear models, Wager et al. (2014) and Mentch and Hooker (2016) address similar problems for random forests.

Sample Splitting. The oldest method for inference after model selection is sample splitting: half the data $D_1$ are used for model fitting and the other half $D_2$ are used for inference.\(^1\)

Thus $S = w_n(D_1)$. The earliest references for sample splitting that we know of are Barnard (1974), Cox (1975), Faraway (1995) Hartigan (1969), page 13 of Miller (1990) Moran (1973), page 37 of

\(^1\) For simplicity, we assume that the data are split into two parts of equal size. The problem of determining the optimal size of the split is not considered in this paper. Some results on this issue are contained in Shao (1993).
Mosteller and Tukey (1977) and Picard and Berk (1990). To quote Barnard: “... the simple idea of splitting a sample in two and then developing the hypothesis on the basis of one part and testing it on the remainder may perhaps be said to be one of the most seriously neglected ideas in statistics ...”

To the best of our knowledge there are only two methods that achieve asymptotically honest coverage: sample splitting and uniform inference. Uniform inference is based on estimating the distribution of the parameter estimates over all possible model selections. In general, this is infeasible. But we compare sample splitting and uniform inference in a restricted model in Section 3.

1.2 Outline

In Section 2 we introduce the basic sample splitting strategies. In Section 3 we compare sample splitting to non-splitting strategies. Section 4 contains some comments on other methods. In Section 5 we report some numerical examples. In Section 6 we establish a Berry-Esseen bound for regression with possibly increasing dimension and no assumption of linearity on the regression function. Section 7 contains concluding remarks. Extra results, proofs and a discussion of another version of the bootstrap, are relegated to the Appendices.

1.3 Notation

Let \( Z = (X, Y) \sim P \) where \( Y \in \mathbb{R} \) and \( X \in \mathbb{R}^d \). We write \( X = (X(1), \ldots, X(d)) \) to denote the components of the vector \( X \). Define \( \Sigma = \mathbb{E}[XX^\top] \) and \( \alpha = (\alpha(1), \ldots, \alpha(d)) \) where \( \alpha(j) = \mathbb{E}[YX(j)] \).

Let \( \sigma = \text{vec}(\Sigma) \) and \( \psi \equiv \psi(P) = (\sigma, \alpha) \). The regression function is \( \mu(x) = \mathbb{E}[Y|X=x] \). We use \( \nu \) to denote Lebesgue measure. We write \( a_n \preceq b_n \) to mean that there exists a constant \( C > 0 \) such that \( a_n \leq C b_n \) for all large \( n \).

For a non-empty subset \( S \subset \{1, \ldots, d\} \) of the covariates \( X_S \) or \( X(S) \) denotes the corresponding elements of \( X \): \( (X(j) : j \in S) \). Similarly, \( \Sigma_S = \mathbb{E}[X_S X_S^\top] \) and \( \alpha_S = \mathbb{E}[YX_S] \).

Let \( \Omega = \Sigma^{-1} \) and \( \omega = \text{vec}(\Omega) \) where \( \text{vec} \) is the operator that stacks a matrix into one large vector. Also, \( \text{vech} \) is the half-vectorization operator that takes a symmetric matrix and stacks the elements on and below the diagonal into a matrix. \( A \otimes B \) denotes the Kronecker product of matrices. The commutation matrix \( K_{m,n} \) is the \( mn \times mn \) matrix defined by \( K_{m,n} \text{vec}(A) = \text{vec}(A^\top) \).

For any \( k \times k \) matrix \( A \), \( \text{vech}(A) \) denotes the column vector of dimension \( k(k+1)/2 \) obtained by vectorizing only the lower triangular part of \( k \times k \) matrix \( A \).

2 Main Results

We now describe how to construct estimators of the random parameters defined earlier. Recall that we rely on data splitting: we randomly split the \( 2n \) data into two halves \( D_{1,n} \) and \( D_{2,n} \). Then, for a given choice of the model selection and estimation rule \( w_n \), we use \( D_{1,n} \) to select a non-empty set of variables \( \hat{S} \subset \{1, \ldots, d\} \) where \( k = |\hat{S}| < n \). For the LOCO and prediction parameters, based on \( D_{1,n} \), we also compute \( \hat{\beta}_{\hat{S}} \), any estimator of the projection parameters restricted to \( \hat{S} \). In addition,
for each $j \in \hat{S}$, we further compute, still using $D_{1,n}$ and the rule $w_n$, $\hat{\beta}_{S(j)}$, the estimator of the projection parameters over the set $\hat{S}(j)$. Also, for $l = 1, 2$, we denote with $I_{l,n}$ random subset of \{1, \ldots, 2n\} containing the indexes for the data points in $D_{l,n}$.

### 2.1 Projection Parameters

In this section we will derive various statistical guarantees for the projection parameters, defined in (1). We will first define the class of data generating distributions on $\mathbb{R}^{d+1}$ for which our results hold. In the definition below, $S$ denotes a non-empty subset of \{1, \ldots, d\} and $W_S = (\text{vech}(X_S X_S^\top), X_S Y)$.

**Definition 1.** Let $\mathcal{P}_{n}^{\text{OLS}}$ be the set of all probability distributions $P$ on $\mathbb{R}^{d+1}$ with zero mean, Lebesgue density and such that, for some positive quantities $A, a, u, U, v$ and $\overline{v}$,

1. the support of $P$ is contained in $[-A, A]^{d+1}$;
2. $\min_{\{S: |S| \leq k\}} \lambda_{\min}(\Sigma_S) \geq u$ and $\max_{\{S: |S| \leq k\}} \lambda_{\max}(\Sigma_S) \leq U$, where $\Sigma_S = \mathbb{E} P[X_S X_S^\top]$;
3. $\min_{\{S: |S| \leq k\}} \lambda_{\min}(\text{Var}_P(W_S)) \geq v$ and $\max_{\{S: |S| \leq k\}} \lambda_{\max}(\text{Var}_P(W_S)) \leq \overline{v}$.
4. $\min\{U, \overline{v}\} \geq \eta$, for a fixed $\eta > 0$.

The first compactness assumption can be easily modified by assuming instead that $Y$ and $X$ are sub-Gaussian, without any technical difficulty. We make such boundedness assumption to simplify our results. The bound on the smallest eigenvalue of $\Sigma_S$, uniformly over all subsets $S$ is natural: the projection parameter is only well defined provided that $\Sigma_S$ is invertible for all $S$, and the closer $\Sigma_S$ is to being singular the higher the uncertainty. The uniform condition on the largest eigenvalue of $\Sigma_S$ in part 2. is used to obtain sharper bounds than the ones stemming from the crude bound $U \leq Ak$ implied by the assumption of a compact support (see e.g. Theorem 1 below). The quantities $v$ and $\overline{v}$ in part 3. are akin to 4th moment conditions. In particular, one can always take $\overline{v} \leq A^2 k^2$ in the very worst case. Finally, the assumption of zero mean is imposed out of convenience and to simplify our derivations, so that we need not to be concerned with an intercept term. As remarked above, in all of our results we have kept track of the dependence on the constants $a, u, U, v$ and $\overline{v}$, so that we may in fact allow all these quantities to change with $n$ (but we do treat $A$ as fixed and therefore have incorporate it in the constants). Finally, the assumption that $tU$ and $\overline{v}$ are bounded from zero is extremely mild. In particular, the parameter $\eta$ is kept fixed and its value affect the constants in Theorems 1, 2 and 4 (the matrix Bernstein inequality (see Lemma 25)).

**Remark.** Although our assumptions imply that the individual coordinates of $X$ are sub-Gaussians, we do not require $X$ itself to be a sub-Gaussian vector, in the usual sense that, for each $d$-dimensional unit vector $\theta$, the random variable $\theta^\top X$ is sub-Gaussian with variance parameter independent of $\theta$ and $d$.

Recall that the projection parameters defined in (1) are

$$
\beta_{S} = \Sigma_{S}^{-1} \alpha_{S},
$$

(8)
We express both the projection parameter \( \beta \) and the model selected based on \( D_{1,n} \) (of size no larger than \( k \)) and
\[
\alpha_{\hat{S}} = \mathbb{E}[YX(\hat{S})] \quad \text{and} \quad \Sigma_{\hat{S}} = \mathbb{E}[X(\hat{S})X(\hat{S})^\top].
\] (9)

We will be studying the ordinary least squares estimator \( \hat{\beta}_{\hat{S}} \) of \( \beta_{\hat{S}} \) computed using the sub-sample \( D_{2,n} \) and restricted to the coordinates \( \hat{S} \). That is,
\[
\hat{\beta}_{\hat{S}} = \Sigma_{\hat{S}}^{-1}\alpha_{\hat{S}}
\] (10)
where, for any non-empty subset \( S \) of \( \{1, \ldots, d\} \),
\[
\alpha_S = \frac{1}{n} \sum_{i \in I_{2,n}} Y_i X_i(S) \quad \text{and} \quad \Sigma_S = \frac{1}{n} \sum_{i \in I_{2,n}} X_i(\hat{S})X_i(S)^\top.
\] (11)

Since each \( P \in \mathcal{P}^\text{OLS}_n \) has a Lebesgue density, \( \Sigma_{\hat{S}} \) is invertible almost surely as long as \( n \geq k \geq |\hat{S}| \). Notice that \( \hat{\beta}_{\hat{S}} \) is not an unbiased estimator of \( \beta_{\hat{S}} \), conditionally or unconditionally on \( D_{2,n} \).

In order to relate \( \hat{\beta}_{\hat{S}} \) to \( \beta_{\hat{S}} \), it will first be convenient to condition on \( \hat{S} \) and thus regard \( \beta_{\hat{S}} \) as a \( k \)-dimensional deterministic vector of parameters (recall that, for simplicity, we assume that \( |\hat{S}| \leq k \), which depends on some unknown \( P \in \mathcal{P}^\text{OLS}_n \). Then, \( \hat{\beta}_{\hat{S}} \) is an estimator of a fixed parameter \( \beta_{\hat{S}} = \beta_{\hat{S}}(P) \) computed using an i.i.d. sample \( D_{2,n} \) from the same distribution \( P \in \mathcal{P}^\text{OLS}_n \). Since all our bounds depend on \( \hat{S} \) only through its size \( k \), those bounds will hold also unconditionally.

For each \( P \in \mathcal{P}^\text{OLS}_n \), we can represent the parameters \( \Sigma_{\hat{S}} = \Sigma_{\hat{S}}(P) \) and \( \alpha_{\hat{S}} = \alpha_{\hat{S}}(P) \) in (9) in vectorized form as
\[
\psi = \psi_{\hat{S}} = \psi(\hat{S}, P) = \begin{bmatrix} \text{vech}(\Sigma_{\hat{S}}) \\ \alpha_{\hat{S}} \end{bmatrix} \in \mathbb{R}^b,
\] (12)
where \( b = \frac{k^2+3k}{2} \). Similarly, based on the sub-sample \( D_{2,n} \) we define the \( n \) random vectors
\[
W_i = \begin{bmatrix} \text{vech}(X_i(\hat{S})X_i(\hat{S})^\top) \\ Y_i \cdot X_i(\hat{S}) \end{bmatrix} \in \mathbb{R}^b, \quad i \in I_{2,n},
\]
and their average
\[
\hat{\psi} = \hat{\psi}_{\hat{S}} = \frac{1}{n} \sum_{i \in I_{2,n}} W_i.
\] (13)

It is immediate to see that \( \mathbb{E}_P[\hat{\psi}] = \psi \), uniformly over all \( P \in \mathcal{P}^\text{OLS}_n \).

We express both the projection parameter \( \beta_{\hat{S}} \) and the least square estimator \( \hat{\beta}_{\hat{S}} \) as non-linear functions of \( \psi \) and \( \hat{\psi} \), respectively, in the following way. Let \( g : \mathbb{R}^b \to \mathbb{R}^k \) be given by
\[
x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto (\mathbb{M}(x_1))^{-1} x_2,
\] (14)
where \( x_1 \) and \( x_2 \) correspond to the first \( k(k+1)/2 \) and the last \( k \) coordinates of \( x \), respectively, and \( \mathbb{M} \) is the inverse mapping of vech, i.e. \( \mathbb{M}(x) = A \) if and only if \( \text{vech}(A) = x \). Notice that \( g \) is well-defined over the convex set
\[
\left\{ \begin{bmatrix} \text{vech}(\Sigma) \\ x \end{bmatrix} : \Sigma \in \mathcal{C}_k^+, x \in \mathbb{R}^k \right\}
\]
where $C_k^+$ is the cone of positive definite matrices of dimension $k$. It follows from our assumptions that, for each $P \in P_n^{\text{OLS}}$, $\psi$ is in the domain of $g$ and, as long as $n \geq d$, so is $\hat{\psi}$, almost surely. Thus, we may write

$$
\beta_{\hat{S}} = g(\psi_{\hat{S}}) \quad \text{and} \quad \hat{\beta}_{\hat{S}} = g(\hat{\psi}_{\hat{S}}).
$$

This formulation of $\beta_{\hat{S}}$ and $\hat{\beta}_{\hat{S}}$ is convenient because, by expanding each coordinate of $g(\hat{\psi})$ separately through a first-order Taylor series expansion around $\psi$, it allows us to re-write $\hat{\beta}_{\hat{S}} - \beta_{\hat{S}}$ as a linear transformation of $\hat{\psi} - \psi$ given by the Jacobian of $g$ at $\psi$, plus a stochastic reminder term. Since $\hat{\psi} - \psi$ is an average, such approximation is simpler to analyze that the original quantity $\hat{\beta}_{\hat{S}} - \beta_{\hat{S}}$ and, provided that the reminder term of the Taylor expansion be small, also sufficiently accurate. This program is carried out in detail and greater generality in a later Section 6, where we derive finite sample Berry-Esseen bounds for non-linear statistics of sums of independent random vectors. The results in this section are direct, albeit non-trivial, applications of those bounds.

**Concentration of $\hat{\beta}_{\hat{S}}$**

We begin by deriving high probability concentration bonds for $\hat{\beta}_{\hat{S}}$ around $\beta_{\hat{S}}$. When there is no model selection nor sample splitting – so that $\hat{S}$ is deterministic and equal to $\{1, \ldots, d\}$ – our results yield consistency rates for the ordinary least squares estimator of the projection parameters, under increasing dimensions and a misspecified model. An analogous result was established in Hsu et al. (2014), where the approximation error $\mu(x) - x^T \beta$ is accounted for explicitly.

**Theorem 1.** Let

$$
B_n = \frac{k}{u^2} \sqrt{U \log k + \log n},
$$

and assume that $\max\{B_n, uB_n\} \to 0$ as $n \to \infty$. Then, there exists a constant $C > 0$, dependent on $A$ and $\eta$ only, such that, for all $n$ large enough,

$$
\sup_{w_n \in W_n} \sup_{P \in P_n^{\text{OLS}}} \|\hat{\beta}_{\hat{S}} - \beta_{\hat{S}}\| \leq CB_n,
$$

with probability at least $1 - \frac{2}{n}$.

**Remarks.**

1. It is worth recalling that, in the result above as well as in all the result of the paper, the probability is with respect to joint distribution of the entire sample and of the splitting process.

2. For simplicity, we have phrased the bound in Theorem 1 in an asymptotic manner. The result can be trivially turned into a finite sample statement by appropriately adjusting the value of the constant $C$ depending on how rapidly $\max\{B_n, uB_n\} \to 0$ vanishes.

3. The proof of the above theorem relies namely an inequality for matrix norms and the vector and matrix Bernstein concentration inequalities (see Lemma 25 below).
4. Theorems 21 and 1 can be easily generalized to cover the case in which the model selection and the computation of the projection parameters are performed on the entire dataset and not on separate, independent splits. In this situation, it is necessary to obtain a high probability bound for the quantity
\[ \max_S \| \beta_S - \hat{\beta}_S \| \]
where the maximum is over all non-empty subsets of \( \{1, \ldots, d\} \) of size at most \( k \) and \( \hat{\beta}_S = \hat{\Sigma}_S^{-1}\hat{\alpha}_S \) (see Equation 11). Since there are less than \( \left( \frac{ed}{k} \right)^k \) such subsets, an additional union bound argument in each application of the matrix and vector Bernstein’s inequalities (see Lemma 25) within the proofs of both Theorem 21 and 1 will give the desired result. The rates so obtained will be then worse than the ones from Theorems 21 and 1 which, because of the sample splitting do not require a union bound. In particular, the scaling of \( k \) with respect to \( n \) will be worse by a factor of \( k \log \frac{d}{k} \). This immediately gives a rate of consistency for the projection parameter under arbitrary model selection rules without relying on sample splitting. We omit the details.

**Confidence sets for the projection parameters: Normal Approximations**

We will now derive confidence intervals for the projection parameters using on a high-dimensional Normal approximation to \( \hat{\beta}_S \). The construction of such confidence sets entails approximating the dominant linear term in the Taylor series expansion of \( \hat{\beta}_S - \beta_S \) by a centered Gaussian vector in \( \mathbb{R}^\hat{S} \) with the same covariance matrix \( \hat{\Gamma}_S \) (see (56) in Section 6). The coverage properties of the resulting confidence sets depend crucially on the ability to estimate such covariance. For that purpose, we use a plug-in estimator, given by
\[ \hat{\Gamma}_S = \hat{G}_S \hat{V}_S \hat{G}_S^\top \]  
where \( \hat{V}_S = \frac{1}{n} \sum_{i=1}^n [(W_i - \hat{\psi})(W_i - \hat{\psi})^\top] \) is the \( b \times b \) empirical covariance matrix of the \( W_i \)’s and the \( k \times b \) matrix \( \hat{G}_S \) is the Jacobian of the mapping \( g \), given explicitly below in (109), evaluated at \( \hat{\psi} \).

The first confidence set for the projection parameter based on the Normal approximation that we propose is an \( L_{\infty} \) ball of appropriate radius centered at \( \hat{\beta}_S \):
\[ \hat{C}_S = \left\{ \beta \in \mathbb{R}^k : \| \beta - \hat{\beta}_S \|_{\infty} \leq \frac{\hat{t}_\alpha}{\sqrt{n}} \right\}, \]  
where \( \hat{t}_\alpha \) is a random radius (dependent on \( D_{2,n} \)) such that
\[ P \left( \| \hat{\Gamma}_S^{1/2} Q \|_{\infty} \leq \hat{t}_\alpha \right) = \alpha, \]  
with \( Q \) a random vector having the \( k \)-dimensional standard Gaussian distribution and independent of the data.

In addition to the \( L_{\infty} \) ball given in (17), we also construct a confidence set for \( \beta_S \) to be a hyper-rectangle, with sides of different lengths in order to account for different variances in the covariates. This can be done using the set
\[ \hat{C}_S = \bigotimes_{j \in \hat{S}} \hat{C}(j), \]  

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where
\[
\tilde{C}(j) = \left[ \beta_S(j) - z_{\alpha/(2k)} \sqrt{\frac{\hat{\Gamma}_S(j,j)}{n}} \beta_S(j) + z_{\alpha/(2k)} \sqrt{\frac{\hat{\Gamma}_S(j,j)}{n}} \right],
\]
with \( \hat{\Gamma}_S \) given by (16) and \( z_{\alpha/(2k)} \) the upper \( 1 - \alpha/(2k) \) quantile of a standard Normal variate. Notice that we use a Bonferroni correction to guarantee a nominal coverage of \( 1 - \alpha \).

**Theorem 2.** Let \( \tilde{C}_S \) and \( \tilde{C}_S \) the confidence sets defined in (17) and (19), respectively. Let
\[
u_n = u - K_{2,n},
\]
where
\[
K_{2,n} = C A \sqrt{k U \log k + \log n/n},
\]
with \( C = C(\eta) > 0 \) the universal constant in (104). Assume, in addition, that \( n \) is large enough so that \( u_n \) is positive. Then, for a \( C > 0 \) dependent on \( A \) only,
\[
\inf_{w_n \in W_n} \inf_{P_n \in P_{n,OLS}} P(\beta \in \tilde{C}_S) \geq 1 - \alpha - C \left( \Delta_{n,1} + \Delta_{n,2} + \Delta_{n,3} \right) \quad (21)
\]
and
\[
\inf_{w_n \in W_n} \inf_{P_n \in P_{n,OLS}} P(\beta \in \tilde{C}_S) \geq 1 - \alpha - C \left( \Delta_{n,1} + \Delta_{n,2} + \tilde{\Delta}_{n,3} \right), \quad (22)
\]
where
\[
\Delta_{n,1} = \left( \frac{\pi^2 k^2 (\log kn)^7}{n^3} \right)^{1/6}, \quad \Delta_{n,2} = \frac{U}{\sqrt{\frac{\pi}{\nu}} \sqrt{k^4 \log^2 n \log k}} \frac{u_n^6}{n^6},
\]
\[
\Delta_{n,3} = \left( \frac{U^2}{\nu} \right)^{1/3} \left( \frac{\nu^2 k^5}{u_n^6 u^4} \frac{\log n}{n} \log^4 k \right)^{1/6} \quad \text{and} \quad \tilde{\Delta}_{n,3} = \min \left\{ \Delta_{n,3}, \frac{U^2}{\nu} \frac{k^5/2}{u_n^6 u^2} \frac{\log n}{n} \log k \right\}.
\]

A few remarks are in order.

1. The coverage probability is affected by three factors: the term \( \Delta_{n,1} \), which bounds the approximation error stemming from the high dimensional Berry-Esseen theorem (see Theorem 27); the term \( \Delta_{n,2} \), which is a high probability bound on the size of the reminder term in the Taylor series expansion of \( \beta_S \) around \( \hat{\beta}_S \) and can therefore be thought of as the price for the non-linearity of the projection parameter, and the terms \( \Delta_{n,3} \) and \( \tilde{\Delta}_{n,3} \), which are due to the fact that the covariance of the estimator is unknown and needs to be also estimated, leading to another source of error (the bootstrap procedure, described below, implicitly estimates this covariance).

2. In terms of dependence of \( k \) on \( n \), all other things being equal, the covariance term \( \Delta_{3,n} \) exhibit the worst rate, as it constrain \( k \) to be of smaller order than \( n^{1/5} \) in order to guarantee asymptotic coverage of \( \tilde{C}_S \). This same term also contains the worst dependence on \( u \), the uniform bound on the smallest eigenvalue of all covariance matrices of the form \( \Sigma_S \), for \( S \subset \{1, \ldots, d\} \) with \( 0 < S \leq k \). Thus, the dependence of the rates on the dimension and on the minimal eigenvalue is overall quite poor. While this is, to an extent, unavoidable, we do not know whether our upper bounds are sharp.
3. The reasons for replacing $u$ by the smaller term $u_n$ given in (20) are somewhat technical, but are explained in the proof of the theorem. Assuming a scaling in $n$ that guarantees that the error terms $\Delta_{1,n}$, $\Delta_{2,n}$ and $\Delta_{3,n}$ are vanishing, such modification is inconsequential and does not affect the rates.

4. The coverage rates obtained for the LOCO and prediction parameters below in Section 2.2 are significantly faster than the ones for the projection parameters, and hold under less restrictions on the class of data generating distributions. We regard this as another reason to prefer the LOCO parameters.

5. Interesting, the covariance error term $\tilde{\Delta}_{3,n}$ for confidence set $\tilde{C}_{\hat{S}}$ is no worse than the corresponding term for the set $\hat{C}_{\hat{S}}$, suggesting that using hyper-rectangles in stead of hyper-cubes may be a better choice.

6. The quantity $\overline{v}$ can of be order $k^2$ in the worst case, further inflating the terms $\Delta_{3,n}$ and $\tilde{\Delta}_{3,n}$.

7. As a function of sample size, there is a term of order $n^{-1/6}$ in $\Delta_{1,n}$ and $\Delta_{3,n}$. The exponent $1/6$ comes from the Berry-Esseen bound in Section 3. Chernozhukov et al. (2014) conjecture that this rate is optimal for high-dimensional central limit theorems. Their conjecture is based on the lower bound result in Bentkus (1985). If their conjecture is true, then this is best rate that can be hoped for in general.

8. The rates are slower than the rate obtained in the central limit theorem given in Portnoy (1987) for robust regression estimators. A reason for such discrepancy is that Portnoy (1987) assumes, among the other things, that the linear model is correct. In this case, the least squares estimators is conditionally unbiased. Without the assumption of model correctness there is a substantial bias.

9. If we assume that the covariates are independent then the situation gets dramatically better. For example, the term $\Delta_{n,2}$ is then $O(1/\sqrt{n})$. But the goal of this paper is to avoid adding such assumptions.

We now consider the accuracy of the confidence set given by the hyper-rectangle $\tilde{C}_{\hat{S}}$ from Equation (19) by deriving an upper bound on the length of the largest side of $\max_{j \in \hat{S}} \tilde{C}(j)$. Similar rates can be obtained for length of the sides of the hyper-cube confidence set $\hat{C}_{\hat{S}}$ given in (17).

**Corollary 3.** With probability at least $1 - \frac{2}{n}$, the maximal length of the sides of the hyper-rectangle $\tilde{C}_{\hat{S}}$ is bounded by

$$C \sqrt{\frac{\log k}{n}} \left( \frac{k^{5/2}}{u_n^3 u^2} \sqrt{\log n} + \frac{k}{u^2} \right),$$

for a constant $C > 0$ depending on $A$ only, uniformly over all $P \in \mathcal{P}_{n,\text{OLS}}$.

**Confidence sets for the projection parameters: The Bootstrap**

The confidence set in (17) based on the Normal approximation require the evaluation of both the matrix $\hat{\Gamma}_{\hat{S}}$ and the quantile $\hat{t}_\alpha$ in (18), which may be computationally inconvenient. Similarly the hyper-rectangle (19) requires computing the diagonal entries in $\hat{\Gamma}_{\hat{S}}$. Below we show that the paired
bootstrap can be deployed to construct analogous confidence sets, centered at \( \hat{\beta}_S \), without knowledge of \( \bar{\Gamma}_S \).

Throughout, by the bootstrap distribution we mean the empirical probability measure associated to the sub-sample \( D_{2,n} \) and conditionally on \( D_{1,n} \) and the outcome of the sample splitting procedure.

We let \( \hat{\beta}^*_S \) denote the estimator of the projection parameters \( \beta_S \) of the form (8) and arising from an i.i.d. sample of size \( n \) drawn from the bootstrap distribution. It is important to point out that \( \hat{\beta}^*_S \) is well-defined only provided that the bootstrap realization of the covariates \( (X_1^*, \ldots, X_n^*) \) is such that the corresponding \( k \)-dimensional empirical covariance matrix

\[
\frac{1}{n} \sum_{i \in D_{2,n}} X_i^*(\hat{S})(X_i^*(\hat{S}))^T
\]

is invertible. Since the data distribution is assumed to have a \( d \)-dimensional Lebesgue density, this occurs almost surely with respect to the distribution of the full sample \( D_n \) if the bootstrap sample contains more than \( k \) distinct values. Thus, the bootstrap guarantees given below only holds on such event. Luckily, this is a matter of little consequence, since under our assumptions the probability that such event does not occur is exponentially small in \( n \) (see Lemma 23 below).

For a given \( \alpha \in (0, 1) \), let \( \hat{\tau}^*_\alpha \) be the smallest positive number such that

\[
P\left( \sqrt{n} \left\| \hat{\beta}^*_S - \beta_S \right\| \leq \hat{\tau}^*_\alpha \left| D_{2,n} \right. \right) \geq 1 - \alpha.
\]

Next, let \((\hat{\tau}^*_j, j \in \hat{S})\) be such that

\[
P\left( \sqrt{n} |\hat{\beta}^*_S(j) - \beta_S(j)| \leq \hat{\tau}^*_j, \forall j \left| D_{2,n} \right. \right) \geq 1 - \alpha.
\]

By the union bound, each \( \hat{\tau}^*_j \) can be chosen to be the largest positive number such that

\[
P\left( \sqrt{n} |\hat{\beta}^*_S(j) - \beta_S(j)| > \hat{\tau}^*_j, \left| D_{2,n} \right. \right) \leq \frac{\alpha}{k}.
\]

Consider the following two bootstrap confidence sets:

\[
\hat{C}^*_S = \left\{ \beta \in \mathbb{R}^\hat{S}: \left\| \beta - \hat{\beta}_S \right\| \leq \frac{\hat{\tau}^*_\alpha}{\sqrt{n}} \right\} \quad \text{and} \quad \tilde{C}^*_S = \left\{ \beta \in \mathbb{R}^\hat{S}: |\beta(j) - \hat{\beta}_S(j)| \leq \frac{\hat{\tau}^*_j}{\sqrt{n}}, \forall j \in \hat{S} \right\}
\]

(23)

It is immediate to see that \( \hat{C}^*_S \) and \( \tilde{C}^*_S \) are just the bootstrap equivalent of the confidence sets of (17) and (19), respectively.

**Theorem 4.** Let

\[
v_n = v - K_{1,n}, \quad \nu_n = \nu + K_{1,n}, \quad u_n = u - K_{2,n} \quad \text{and} \quad U_n = U + K_{2,n},
\]

where

\[
K_{1,n} = CA^2 \sqrt{bv \log b + \log n \over n} \quad \text{and} \quad K_{2,n} = CA \sqrt{kU \log k + \log n \over n},
\]

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with \( C = C(\eta) > 0 \) the constant in (104). Assume that \( n \) is large enough so that \( v_n = v - K_{1,n} \) and \( u_n = u - K_{2,n} \) are both positive. Then, for a constant \( C = C(A) > 0 \),

\[
\inf_{u_n \in W_n} \inf_{P \in P_{OLS}} P(\beta_S^* \in C_S^*) \geq 1 - \alpha - C(\Delta_{n,1}^* + \Delta_{n,2}^* + \Delta_{n,3}^*) ,
\]

(24)

where \( C_S^* \) is either one of the bootstrap confidence sets in (23),

\[
\Delta_{n,1}^* = \frac{1}{\sqrt{v_n}} \left( \frac{2^2 v_n^2 (\log kn)^7}{n} \right)^{1/6} , \quad \Delta_{n,2}^* = \frac{U_n}{\sqrt{v_n}} \left( \frac{k^4 v_n \log^2 n \log k}{n u_n^6} \right)
\]

and \( \Delta_{n,3}^* \) is as in Theorem 2.

**Remark.** The term \( \Delta_{n,3}^* \) remains unchanged from the Normal approximating case since it arises from the Gaussian comparison part, which does not depend on the bootstrap distribution.

**Remark.** It is important that we use the pairs bootstrap — where each pair \( Z_i = (X_i, Y_i), i = I_{2,n} \), is treated as one observation — rather than a residual based bootstrap. In fact, the validity of the residual bootstrap requires the underlying regression function to be linear, which we do not assume. See Buja et al. (2015) for more discussion on this point. In both cases, the Berry-Esseen theorem for simple convex sets (polyhedra with a limited number of faces) with increasing dimension due to Chernozhukov et al. (2013, 2014) justifies the method. In the case of \( \beta_S^* \) we also need a Taylor approximation followed by an application of the Gaussian anti-concentration result from the same reference.

The coverage rates from Theorem 4 are of course no better than the ones obtained in Theorem 2, and are consistent with the results of El Karoui and Purdom (2015) who found that, even when the linear model is correct, the bootstrap does poorly when \( k \) increases.

The coverage accuracy can also be improved by changing the bootstrap procedure; see Section 8.

**Remark.** Our results concern the bootstrap distribution and assume the ability to determine the quantities \( \tilde{t}_a^* \) and \( (\tilde{t}_j^*, j \in \hat{S}) \) in Equation (23). Of course, they can be approximated to an arbitrary level of precision by drawing a large enough number \( B \) of bootstrap samples and then by computing the appropriate empirical quantiles from those samples. This will result in an additional approximation error, which can be easily quantified using the DKW inequality (and, for the set \( \tilde{C}_S^* \), also the union bound) and which is, for large \( B \), negligible compared to the size of the error bounds obtained above. For simplicity, we do not provide these details. Similar considerations apply to all subsequent bootstrap results.

**The Sparse Case**

Now we briefly discuss the case of sparse fitting where \( k = O(1) \) so that the size of the selected model is not allowed to increase with \( n \). In this case, things simplify considerably. The standard central limit theorem shows that

\[ \sqrt{n}(\hat{\beta} - \beta) \sim N(0, \Gamma) \]
where $\Gamma = \Sigma^{-1}E[(Y - \beta^TX)^2]\Sigma^{-1}$. Furthermore, $\Gamma$ can be consistently estimated by the sandwich estimator $\hat{\Gamma} = \hat{\Sigma}^{-1}A\hat{\Sigma}^{-1}$ where $A = n^{-1}X^TRX$, $X_{ij} = X_i(j)$, $R$ is the $k \times k$ diagonal matrix with $R_{ii} = (Y_i - X_i^T\beta)^2$. By Slutsky’s theorem, valid asymptotic confidence sets can be based on the Normal distribution with $\hat{\Gamma}$ in place of $\Gamma$ (Buja et al. (2015)).

However, if $k$ is non-trivial relative to $n$, then fixed $k$ asymptotics may be misleading. In this case, the results of the previous section may be more appropriate. In particular, replacing $\Gamma$ with an estimate then has a non-trivial effect on the coverage accuracy. Furthermore, the accuracy depends on $1/u$ where $u = \lambda_{\min}(\Sigma)$. But when we apply the results after sample splitting (as is our goal), we need to define $u$ as $u = \min|S|\leq k \lambda_{\min}(\Sigma_S)$. As $d$ increases, $u$ can get smaller and smaller even with fixed $k$. Hence, the usual fixed $k$ asymptotics may be misleading.

**Remark:** We only ever report inferences for the selected parameters. The bootstrap provides uniform coverage over all parameters in $S$. There is no need for a Bonferroni correction. This is because the bootstrap is applied to $||\hat{\beta}_S - \beta_S||_\infty$. However, we also show that univariate Normal approximations together with Bonferroni adjustments leads valid hyper-rectangular regions; see Theorem 19.

### 2.2 LOCO Parameters

Now we turn to the LOCO parameter $\gamma_\hat{S} \in \mathbb{R}^{\hat{S}}$, where $\hat{S}$ is the model selected on the first half of the data. Recall that $j^{th}$ coordinate of this parameter is

$$\gamma_\hat{S}(j) = \mathbb{E}_{X,Y} \left[ |Y - \hat{\beta}_S^T X_{\hat{S}(j)}| - |Y - \hat{\beta}_{\hat{S}}^T X_{\hat{S}}| \right]_{D_{1,n}},$$

where $\hat{\beta}_S \in \mathbb{R}^{\hat{S}}$ is any estimator of $\beta_S$, and $\hat{\beta}_{\hat{S}(j)}$ is obtained by re-computing the same estimator on the set of covariates $\hat{S}(j)$ resulting from re-running the same model selection procedure after removing covariate $X_j$. The model selections $\hat{S}$ and $\hat{S}(j)$ and the estimators $\hat{\beta}_S$ and $\hat{\beta}_{\hat{S}(j)}$ are all computed using half of the sample, $D_{1,n}$.

In order to derive confidence sets for $\gamma_\hat{S}$ we will assume that the data generating distribution belongs to the class $\mathcal{P}_n$ of all distributions on $\mathbb{R}^{d+1}$ supported on $[-A, A]^{d+1}$, for some fixed constant $A > 0$. Clearly the class $\mathcal{P}_n^{\text{LOCO}}$ is significantly larger then the class $\mathcal{P}_n^{\text{OLS}}$ considered for the projection parameters.

A natural unbiased estimator of $\gamma_\hat{S}$ – conditionally on $D_{1,n}$ – is

$$\hat{\gamma}_\hat{S} = \frac{1}{n} \sum_{i \in I_{2,n}} \delta_i,$$

with $(\delta_i, i \in I_{2,n})$ independent and identically distributed random vectors in $\mathbb{R}^{\hat{S}}$ such that, for any $i \in I_{2,n}$ and $j \in \hat{S}$,

$$\delta_i(j) = \left| Y_i - \hat{\beta}_S^T X_i(\hat{S}(j)) \right| - \left| Y_i - \hat{\beta}_{\hat{S}}^T X_i(\hat{S}) \right|.$$  \hspace{1cm} (25)
To derive a CLT for \( \hat{\gamma}_S \) we face two technical problem. First, we require some control on the minimal variance of the coordinates of the \( \delta_i \)'s. Since we allow for increasing \( k \) and we impose minimal assumptions on the class of data generating distributions, it is possible that any one variable might have a tiny influence on the predictions. As a result, we cannot rule out the possibility that the variance of some coordinate of the \( \delta_i \) vanishes. In this case the rate of convergence in high-dimensional central limit theorems would be negatively impacted, in ways that are difficulty to assess. To prevent such issue we simply redefine \( \hat{\gamma}_S \) by adding a small amount of noise with non-vanishing variance. Secondly, we also need an upper bound on the third moments of the coordinates of the \( \delta_i \)'s. In order to keep the presentation simple, we will truncate the estimator of the regression function by hard-thresholding so that it has bounded range \([-\tau, \tau]\) for a given \( \tau > 0 \). Since both \( Y \) and the coordinates of \( X \) are uniformly bounded in absolute value by \( A \), this assumption is reasonable. Thus, we re-define the vector of LOCO parameters \( \gamma_S \) so that its \( j^{th} \) coordinate is

\[
\gamma_S(j) = \mathbb{E}_{X,Y,\xi_i} \left[ Y - t_\tau \left( \hat{\beta}_S^T X_{\hat{S}(j)} \right) \right] - \left| Y - t_\tau \left( \hat{\beta}_S^T X_{\hat{S}(j)} \right) \right| + \epsilon \xi_i(j),
\]

where \( \epsilon > 0 \) is a pre-specified small number, \( \xi = (\xi(j), j \in \hat{S}) \) is a random vector comprised of independent Uniform\((-1, 1)\), independent of the data, and \( t_\tau \) is the hard-threshold function: for any \( x \in \mathbb{R} \), \( t_\tau(x) = x \) if \( |x| \leq \tau \) and \( \text{sign}(x) \tau \) otherwise. Accordingly, we re-define the estimator \( \hat{\gamma}_S \) of this modified LOCO parameters as

\[
\hat{\gamma}_S = \frac{1}{n} \sum_{i \in I_{2,n}} \delta_i,
\]

where the \( \delta_i \)'s are random vector in \( \mathbb{R}^{\hat{S}} \) such that the \( j^{th} \) coordinate of \( \delta_i \) is

\[
\left| Y_i - t_\tau \left( \hat{\beta}_S^T X_i(\hat{S}(j)) \right) \right| - \left| Y_i - t_\tau \left( Y_i - \hat{\beta}_S^T X_i(\hat{S}) \right) \right| + \epsilon \xi_i(j), \quad j \in \hat{S}.
\]

**Remark.** Introducing additional noise has the effect of making the inference conservative: the confidence intervals will be slightly wider. For small \( \epsilon \) and any non-trivial value of \( \gamma_S(j) \) this will presumably have a negligible effect. For our proofs, adding some additional noise and thresholding the regression function are advantageous because the first choice will guarantee that the empirical covariance matrix of the \( \delta_i \)'s is non-singular, and the second choice will imply that the coordinates of \( \gamma_S \) are bounded. It is possible to let \( \epsilon \to 0 \) and \( \tau \to \infty \) as \( n \to \infty \) at the expense of slower concentration and Berry-Esseen rates. For simplicity, we take \( \epsilon \) and \( \tau \) to be fixed but we will keep explicit track of these quantities in the constants.

Since each coordinate of \( \gamma_S \) is an average of random variables that are bounded in absolute value by \( 2(A + \tau) + \epsilon \), and \( \mathbb{E} \left[ \hat{\gamma}_S | D_{1,n} \right] = \gamma_S \), a standard bound for the maxima of \( k \) bounded (and, therefore, sub-Gaussian) random variables yields the following concentration result. As usual, the probability is with respect to the randomness in the full sample and in the splitting.
Lemma 5.

\[
\sup_{w_n \in W_n} \sup_{P \in P_n^{\text{LOCO}}} \mathbb{P}\left( \| \hat{\gamma}_S - \gamma \|_\infty \leq (2(A + \tau) + \epsilon) \sqrt{\frac{2 \log k + \log n}{n}} \right) \geq 1 - \frac{1}{n}.
\]

Proof. The bound on \( \| \hat{\gamma}_S - \gamma \|_\infty \) holds with probability at least \( 1 - \frac{1}{n} \) conditionally on \( D_{1,n} \) and the outcome of data splitting, and uniformly over the choice of the procedure \( w_n \) and of the distribution \( P \). Thus, the uniform validity of the bound holds also unconditionally.

We now construct confidence sets for \( \gamma \). Just like we did with the projection parameters, we consider two types of methods: one based on Normal approximations and the other on the bootstrap.

**Normal Approximation**

Obtaining high-dimensional Berry-Esseen bounds for \( \hat{\gamma}_S \) is nearly straightforward since, conditionally on \( D_{1,n} \) and the splitting, \( \hat{\gamma}_S \) is just a vector of averages of bounded and independent variables with non-vanishing variances. Thus, there is no need for a Taylor approximation and we can apply directly the results in Chernozhukov et al. (2014). In addition, we find that the accuracy of the confidence sets for this LOCO parameter is higher than for the projection parameters.

Similarly to what we did in Section 2.1, we derive two approximate confidence sets: one is an \( L_\infty \) ball and the other is a hyper-rectangle whose \( j \)th side length is proportional to the standard deviation of the \( j \)th coordinate of \( \hat{\gamma}_S \). Both sets are centered at \( \hat{\gamma}_S \).

Below, we let \( \alpha \in (0,1) \) be fixed and let

\[
\hat{\Sigma}_S = \frac{1}{n} \sum_{i=1}^{n} (\delta_i - \hat{\gamma}_S)(\delta_i - \hat{\gamma}_S)^\top,
\]

be the empirical covariance matrix of the \( \delta_i \)'s. The first confidence set is the \( L_\infty \) ball

\[
\hat{D}_S = \left\{ \gamma \in \mathbb{R}^k : \| \gamma - \hat{\gamma}_S \|_\infty \leq \hat{t}_\alpha \right\},
\]

where \( \hat{t}_\alpha \) is such that

\[
\mathbb{P}\left( \| Z_n \|_\infty \leq \hat{t}_\alpha \right) = 1 - \alpha,
\]

with \( Z_n \sim N(0, \hat{\Sigma}_S) \). The second confidence set we construct is instead the hyper-rectangle

\[
\tilde{D}_S = \bigotimes_{j \in \hat{S}} \tilde{D}(j),
\]

where, for any \( j \in \hat{S} \), \( \tilde{D}(j) = [\tilde{\gamma}_S(j) - \tilde{t}_{j,\alpha}, \tilde{\gamma}_S(j) + \tilde{t}_{j,\alpha}] \), with \( \tilde{t}_{j,\alpha} = z_{\alpha/2k} \sqrt{\frac{\hat{\Sigma}_S(j,j)}{n}} \).

The above confidence sets have the same form as the confidence sets for the projection parameters (65) (68). The key difference is that for the projection parameters we use the estimated covariance
of the linear approximation to \( \hat{\beta}_S \), while for the LOCO parameter \( \hat{\gamma}_S \) we rely on the empirical covariance (28), which is a much simpler estimator to compute.

In the next result we derive coverage rates for both confidence sets.

**Theorem 6.** There exists a universal constant \( C > 0 \) such that

\[
\inf_{w_n \in W_n} \inf_{P \in \mathcal{P}_{n}^{\text{LOCO}}} \mathbb{P} \left( \gamma_S \in \hat{D}_S \right) \geq 1 - \alpha - C \left( E_{1,n} + E_{2,n} \right) - \frac{1}{n},
\]

and

\[
\inf_{w_n \in W_n} \inf_{P \in \mathcal{P}_{n}^{\text{LOCO}}} \mathbb{P} \left( \gamma_S \in \tilde{D}_S \right) \geq 1 - \alpha - C \left( E_{1,n} + \tilde{E}_{2,n} \right) - \frac{1}{n},
\]

where

\[
E_{1,n} = \frac{2(A + \tau) + \epsilon}{\epsilon} \left( \frac{\log nk}{n} \right)^{1/6},
\]

\[
E_{2,n} = \frac{N_n^{1/3}(2 \log 2k)^{2/3}}{\epsilon^{2/3}},
\]

\[
\tilde{E}_{2,n} = \min \left\{ E_{2,n}, \frac{N_n \gamma_{\alpha/(2k)}}{\epsilon^2} \left( \sqrt{2 + \log(2k)} + 2 \right) \right\}
\]

and

\[
N_n = (2(A + \tau) + \epsilon)^2 \sqrt{\frac{4 \log k + 2 \log n}{n}}.
\]

**Remark.** The term \( E_{1,n} \) quantifies the error in applying the high-dimensional normal approximation to \( \hat{\gamma}_S - \gamma_S \), given in Chernozhukov et al. (2014). The second error term \( E_{2,n} \) is due to the fact that \( \Sigma_S \) is unknown and has to be estimated using the empirical covariance matrix \( \hat{\Sigma}_S \). To establish \( E_{2,n} \) we use the Gaussian comparison Theorem 28. We point out that the dependence in \( \epsilon \) displayed in the term \( E_{2,n} \) above does not follow directly from Theorem 2.1 in Chernozhukov et al. (2014). It can be obtained by tracking constants and using Nazarov’s inequality Theorem 26 in the proof of that result. See Theorem 27 in Section 13 for details.

The accuracy of the confidence set (30) can be easily established to be of order \( O \left( \sqrt{\frac{\log k}{n}} \right) \), a fact made precise in the following result.

**Corollary 7.** With probability at least \( 1 - \frac{1}{n} \), the maximal length of the sides of the hyper-rectangle \( C_n \) is bounded by

\[
C \left( 2(A + \tau) + \epsilon \right) \sqrt{\frac{\log k}{n} \left( 1 + \frac{(4 \log k + 2 \log n)^{1/2}}{n^{1/2}} \right)},
\]

for a universal constant \( C > 0 \), uniformly over all \( P \in \mathcal{P}_{n}^{\text{LOCO}} \).
The Bootstrap

We now demonstrate the coverage of the paired bootstrap version of the confidence set for $\gamma_{\hat{S}}$ given above in (29).

The bootstrap distribution is the empirical measure associated to the $n$ triplets $\{(X_i, Y_i, \xi_i), i \in I_{2,n}\}$ and conditionally on $D_{1,n}$. Let $\hat{\gamma}_{\hat{S}}^*$ denote the estimator of the LOCO parameters (26) of the form (27) computed from an i.i.d. sample of size $n$ drawn from the bootstrap distribution. Notice that

$$E\left[\hat{\gamma}_{\hat{S}}^*\right](X_i, Y_i, \xi_i), i \in I_{2,n}\right] = \hat{\gamma}_{\hat{S}}.$$

For a given $\alpha \in (0, 1)$, let $\tilde{t}_\alpha^*$ be the smallest positive number such that

$$P\left(\sqrt{n}\|\gamma_{\hat{S}}^* - \hat{\gamma}_{\hat{S}}\| \leq \tilde{t}_\alpha^*, \left|(X_i, Y_i, \xi_i), i \in I_{2,n}\right) \geq 1 - \alpha.\right.$$

In particular, using the union bound, each $\tilde{t}_\alpha^*$ can be chosen to be the largest positive number such that

$$P\left(\sqrt{n}q_{\hat{S}}^*(j) - \hat{\gamma}_{\hat{S}}(j) > \tilde{t}_j^*, \left|(X_i, Y_i, \xi_i), i \in I_{2,n}\right) \leq \frac{\alpha}{k}.\right.$$

Consider the following two bootstrap confidence sets:

$$\hat{D}_{\hat{S}}^* = \left\{ \gamma \in \mathbb{R}^\hat{S} : \|\gamma - \hat{\gamma}_{\hat{S}}\|_\infty \leq \frac{\tilde{t}_\alpha^*}{\sqrt{n}} \right\} \quad \text{and} \quad \hat{D}_{\hat{S}}^* = \left\{ \gamma \in \mathbb{R}^\hat{S} : |\gamma_j - \hat{\gamma}_j| \leq \frac{\tilde{t}_j^*}{\sqrt{n}}, \forall j \right\}. \quad (37)$$

**Theorem 8.** Using the same notation as in Theorem 6, assume that $n$ is large enough so that $\epsilon_n = \sqrt{\epsilon^2 - N_n}$ is positive. Then there exists a universal constant $C > 0$ such that the coverage of both confidence sets in (37) is at least

$$1 - \alpha - C \left( E_{1,n}^* + E_{2,n} + \frac{1}{n} \right),$$

where

$$E_{1,n}^* = \frac{2(A + \tau) + \epsilon_n}{\epsilon_n} \left( \frac{(\log nk)^7}{n} \right)^{1/6}. \quad (22)$$

### 2.3 Median LOCO parameters

For the median loco parameters $(\phi_{\hat{S}}(j), j \in \hat{S})$ given in (3) finite sample inference is relatively straightforward using standard confidence intervals for the median based on order statistics. In detail, for each $j \in \hat{S}$ and $i \in I_{2,n}$, recall the definition of $\delta_i(j)$ in (25) and let $\delta_{(1)}(j) \leq \cdots \leq \delta_{(n)}(j)$ be the corresponding order statistics. We will not impose any restrictions on the data generating distribution. In particular, for each $j \in \hat{S}$, the median of $\delta_i(j)$ needs not be unique. Consider the interval

$$E_j = [\delta_{(l)}(j), \delta_{(u)}(j)].$$
where
\[ l = \left\lceil \frac{n}{2} - \sqrt{\frac{n}{2} \log \left( \frac{2k}{\alpha} \right)} \right\rceil \quad \text{and} \quad u = \left\lfloor \frac{n}{2} + \sqrt{\frac{n}{2} \log \left( \frac{2k}{\alpha} \right)} \right\rfloor \] (38)

and construct the hyper-cube
\[ \hat{E}_S = \bigotimes_{j \in \hat{S}} E_j. \] (39)

Then, a standard result about confidence sets for medians along with union bound implies that \( \hat{E}_S \) is a \( 1 - \alpha \) confidence set for the median LOCO parameters, uniformly over \( \mathcal{P}_n \).

**Proposition 9.** For every \( n \),
\[
\inf_{w_n \in \mathcal{W}_n} \inf_{P \in \mathcal{P}_n} \mathbb{P}(\phi_S \in \hat{E}_S) \geq 1 - \alpha.
\] (40)

**Remark.** Of course, if the median of \( \delta_i(j) \) is not unique, the length of the corresponding confidence interval does not shrink as \( n \) increases. But if the median is unique for each \( j \in \hat{S} \), and under addition smoothness conditions, we obtain the maximal length the side of the confidence rectangle \( \hat{E}_S \) is of order \( O \left( \sqrt{\log k + \log n} \right) \), with high probability.

**Theorem 10.** Suppose that there exists positive numbers \( M \) and \( \eta \) such that, for each \( j \in \hat{S} \), the cumulative distribution function of each \( \delta_i(j) \) is differentiable with derivative no smaller than \( M \) at all points at a distance no larger than \( \eta \) from its (unique) median. Then, for all \( n \) for which
\[
\frac{1}{n} + \sqrt{\frac{1}{2n} \log \left( \frac{2k}{\alpha} \right)} + \sqrt{\frac{\log 2kn}{2n}} \leq \eta M,
\]
the sides of \( \hat{E}_S \) have length uniformly bounded by
\[
\frac{2}{M} \left( \frac{1}{n} + \sqrt{\frac{1}{2n} \log \left( \frac{2k}{\alpha} \right)} + \sqrt{\frac{\log 2kn}{2n}} \right),
\]
with probability at least \( 1 - \frac{1}{n} \).

### 2.4 Future Prediction Error

To construct a confidence interval for the future prediction error parameter \( \rho_S \) consider the set
\[
\hat{F}_S = \left[ \hat{\rho}_S - z_{\alpha/2} s / \sqrt{n}, \hat{\rho}_S + z_{\alpha/2} s / \sqrt{n} \right]
\]
where \( z_{\alpha/2} \) is the \( 1 - \alpha/2 \) upper quantile of a standard normal distribution,
\[
\hat{\rho}_S = \frac{1}{n} \sum_{i \in \mathcal{I}_2} A_i, \quad s^2 = \frac{1}{n} \sum_{i \in \mathcal{I}_2} (A_i - \hat{\rho}_S)^2, \quad \text{and} \quad A_i = |Y_i - \hat{\beta}_S^\top X_i(\hat{S})|, \forall i \in \mathcal{I}_{2,n}.
\]
For any \( P \), let \( \sigma_n^2 = \sigma_n^2(P) = \text{Var}_P(A_1) \) and \( \mu_{3,n} = \mu_{3,n}(P) = \mathbb{E}_P[|A_1 - \mathbb{E}_P[A_1]|^3] \). Then, by the one-dimensional Berry-Esseen theorem:

\[
\inf_{w_n \in W_n} \mathbb{P}(\rho_{\hat{S}} \in \hat{F}_{\hat{S}}) \geq 1 - \alpha - O\left( \frac{\mu_{3,n}}{\sigma_n \sqrt{n}} \right).
\]

In order to obtain uniform coverage accuracy guarantees, we may rely on a modification of the target parameter that we implemented for the LOCO parameters in Section 2.2 and redefine the prediction parameter to be

\[
\rho_{\hat{S}} = \mathbb{E}\left[ |Y - t_\tau(\hat{\beta}_\tau X(S))| + \epsilon \xi \right],
\]

where \( t_\tau \) is the hard-threshold function (for any \( x \in \mathbb{R}, t_\tau(x) \) is \( x \) if \( |x| \leq \tau \) and \( \text{sign}(x) \tau \) otherwise) and \( \xi \) is independent noise uniformly distributed on \([-1,1]\). Above, the positive parameters \( \tau \) and \( \epsilon \) are chosen to ensure that the variance of the \( A_i \)'s does not vanish and that their third moment does not explode as \( n \) grows. With this modification, we can ensure that \( \sigma_n^2 \geq \epsilon^2 \) and \( \mu_{3,n} \leq (A + \tau + \epsilon)^3 \) uniformly in \( n \) and also \( s \leq 4(A + \tau + \epsilon)^2 \), almost surely. Of course, we may let \( \tau \) and \( \epsilon \) change with \( n \) in a controlled manner. But for fixed choices of \( \tau \) and \( \epsilon \) we obtain the following parametric rate for \( \rho_{\hat{S}} \), which holds for all possible data generating distributions:

\[
\inf_{w_n \in W_n} \mathbb{P}(\rho_{\hat{S}} \in \hat{F}_{\hat{S}}) \geq 1 - \alpha - C\left( \frac{1}{\sqrt{n}} \right),
\]

for a constant dependent only on \( A, \tau \) and \( \epsilon \). Furthermore, the length of the confidence interval is parametric, of order \( \frac{1}{\sqrt{n}} \).

3 Prediction/Accuracy Tradeoff: Comparing Splitting to Uniform Inference

There is a price to pay for sample splitting: the selected model may be less accurate because only part of the data are used to select the model. Thus, splitting creates gains in accuracy and robustness for inference but with a possible loss of prediction accuracy. We call this the inference-prediction tradeoff. In this section we study this phenomenon by comparing splitting with uniform inference (defined below). We use uniform inference for the comparison since this is the any other method we know of that achieves (6). We study this use with a simple model where it is feasible to compare splitting with uniform inference. We will focus on the many means problem which is similar to regression with a balanced, orthogonal design. The data are \( Y_1, \ldots, Y_{2n} \sim P \) where \( Y_i \in \mathbb{R}^D \). Let \( \beta = (\beta(1), \ldots, \beta(D)) \) where \( \beta(j) = \mathbb{E}[Y_i(j)] \). In this section, the model \( \mathcal{P}_n \) is the set of probability distributions on \( \mathbb{R}^D \) such that \( \max_j \mathbb{E}[Y(j)]^3 < C \) and \( \min_j \text{Var}(Y(j)) > c \) for some positive \( C \) and \( c \), which do not change with \( n \) or \( D \) (these assumptions could of course be easily relaxed). Below, we will only track the dependence on \( D \) and \( n \) and will use the notation \( \preceq \) to denote inequality up to constants.

To mimic forward stepwise regression — where we would choose a covariate to maximize correlation with the outcome — we consider choosing \( j \) to maximize the mean. Specifically, we take

\[
\hat{S} \equiv w(Y_1, \ldots, Y_{2n}) = \arg\max_j \overline{Y}(j)
\]

(41)
where $\overline{Y}(j) = (1/2n) \sum_{i=1}^{2n} Y_i(j)$. Our goal is to infer the random parameter $\beta_{\hat{S}}$. The number of models is $D$. In forward stepwise regression with $k$ steps and $d$ covariates, the number of models is $D = d^k$. So the reader is invited to think of $D$ as being very large. We will compare splitting versus non-splitting with respect to three goals: estimation, inference and prediction accuracy.

**Splitting:** In this case we take Let $D_{1,n} = \{i : 1 \leq i \leq n\}$ and $D_{2,n} = \{i : n + 1 \leq i \leq 2n\}$. Then

$$\hat{S} \equiv w(Y_1, \ldots, Y_n) = \arg\max_j \overline{Y}(j) \quad (42)$$

where $\overline{Y}(j) = (1/n) \sum_{i=1}^{2n} Y_i(j)$. The point estimate and confidence interval for the random parameter $\beta_{\hat{S}}$ are

$$\hat{\beta}_{\hat{S}} = \frac{1}{n} \sum_{i=n+1}^{2n} Y_i(\hat{S})$$

and

$$\hat{C}_{\hat{S}} = [\hat{\beta}_{\hat{S}} - sz_{a/2}/\sqrt{n}, \hat{\beta}_{\hat{S}} + sz_{a/2}/\sqrt{n}]$$

where $s^2 = n^{-1} \sum_{i=n+1}^{2n} (Y_i(\hat{S}) - \hat{\beta}_{\hat{S}})^2$.

**Uniform Inference (Non-Splitting).** By “non-splitting” we mean that the selection rule and estimator are invariant under permutations of the data. In particular, we consider uniform inference which is defined as follows. Let $\hat{\beta}(s) = (2n)^{-1} \sum Y_i(s)$ be the average over all the observations. Let $\hat{S} = \arg\max_s \hat{\beta}(s)$. Our point estimate is $\hat{\beta}_{\hat{S}} \equiv \hat{\beta}(\hat{S})$. Now define

$$F_n(t) = \mathbb{P}(\sup_s \sqrt{2n} |\hat{\beta}(s) - \beta(s)| \leq t).$$

We can consistently estimate $F_n$ by the bootstrap:

$$\hat{F}_n(t) = \mathbb{P}(\sup_s \sqrt{2n} |\hat{\beta}^*(s) - \hat{\beta}(s)| \leq t | Y_1, \ldots, Y_{2n}).$$

A valid confidence set for $\beta$ is $R = \{\beta : \|\beta - \hat{\beta}\|_{\infty} \leq t/\sqrt{2n}\}$ where $t = \hat{F}_n^{-1}(1 - \alpha)$. Because this is uniform over all possible models (that is, over all $s$), it also defines a valid confidence interval for a randomly selected coordinate. In particular, we can define

$$\hat{C}_{\hat{S}} = [\hat{\beta}_{\hat{S}} - t/\sqrt{2n}, \hat{\beta}_{\hat{S}} + t/\sqrt{2n}]$$

Both confidence intervals satisfy (6).

We now compare $\hat{\beta}_{\hat{S}}$ and $\hat{C}_{\hat{S}}$ for both the splitting and non-splitting procedures. The reader should keep in mind that, in general, $\hat{S}$ might be different between the two procedures, and hence $\beta_{\hat{S}}$ may be different. The two procedures might be estimating different parameters. We discuss that issue shortly.

**Estimation.** First we consider estimation accuracy.
Lemma 11. For the splitting estimator:

$$\sup_{P \in \mathcal{P}_n} \mathbb{E}|\hat{\beta}_S - \beta_S| \leq n^{-1/2}. \quad (43)$$

For non-splitting we have

$$\inf \sup_{\beta} \mathbb{E}|\hat{\beta}_S - \beta_S| \geq \sqrt{\frac{\log D}{n}}. \quad (44)$$

The above is stated for the particular selection rule \( \hat{S} = \text{argmax}_n \hat{\beta}_s \), but the splitting-based result holds for general selection rules \( w \in \mathcal{W}_n \), so that for splitting

$$\sup_{w \in \mathcal{W}_n} \sup_{P \in \mathcal{P}_n} \mathbb{E}|\hat{\beta}_S - \beta_S| \leq n^{-1/2} \quad (45)$$

and for non-splitting

$$\inf_{\beta} \sup_{w \in \mathcal{W}_2} \sup_{P \in \mathcal{P}_n} \mathbb{E}|\hat{\beta}_S - \beta_S| \geq \sqrt{\frac{\log D}{n}}. \quad (46)$$

Thus, the splitting estimator converges at a \( n^{-1/2} \) rate. Non-splitting estimators have a slow rate, even with the added assumption of Normality. (Of course, the splitting estimator and non-splitting estimator may in fact be estimating different randomly chosen parameters. We address this issue when we discuss prediction accuracy.)

Inference. Now we turn to inference. For splitting, we use the usual Normal interval \( \hat{C}_S = [\hat{\beta}_S - z_{\alpha}s/\sqrt{n}, \hat{\beta}_S + z_{\alpha}s/\sqrt{n}] \) where \( s^2 \) is the sample variance from \( \mathcal{D}_{2,n} \). We then have, as a direct application of the one-dimensional Berry-Esseen theorem, that:

Lemma 12. Let \( \hat{C}_S \) be the splitting-based confidence set. Then,

$$\inf_{P \in \mathcal{P}_n} \mathbb{P}(\beta_S \in \hat{C}_S) = 1 - \alpha - \frac{c}{\sqrt{n}} \quad (47)$$

for some \( c \). Also,

$$\sup_{P \in \mathcal{P}_n} \mathbb{E}[\nu(\hat{C}_S)] \leq n^{-1/2} \quad (48)$$

where \( \nu \) is Lebesgue measure. More generally,

$$\inf_{w \in \mathcal{W}_n} \inf_{P \in \mathcal{P}_n} \mathbb{P}(\beta_S \in \hat{C}_S) = 1 - \alpha - \frac{c}{\sqrt{n}} \quad (49)$$

for some \( c \), and

$$\sup_{w \in \mathcal{W}_n} \sup_{P \in \mathcal{P}_n} \mathbb{E}[\nu(\hat{C}_S)] \leq n^{-1/2} \quad (50)$$

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Lemma 13. Let $\hat{C}_S$ be the uniform confidence set. Then,

$$\inf_{P \in P_n} P(\beta^* \in \hat{C}_S) = 1 - \alpha - \left( c \frac{(\log D)^7}{n} \right)^{1/6}$$

for some $c$. Also,

$$\sup_{P \in P_{2n}} E[\nu(\hat{C}_S)] \geq \sqrt{\frac{\log D}{n}}.$$  \hspace{1cm} (52)

The proof is a straightforward application of results in Chernozhukov et al. (2013, 2014). We thus see that the splitting method has better coverage and narrower intervals, although we remind the reader that the two methods may be estimating different parameters.

**Can We Estimate the Law of $\hat{\beta}(S)$?** An alternative non-splitting method to uniform inference is to estimate the law $F_{2n}$ of $\sqrt{2n}(\hat{\beta}_S - \beta^*_S)$. But we show that the law of $\sqrt{2n}(\hat{\beta}_S - \beta^*_S)$ cannot be consistently estimated even if we assume that the data are Normally distributed and even if $D$ is fixed (not growing with $n$). This was shown for fixed population parameters in Leeb and Pötscher (2008). We adapt their proof to the random parameter case in the following lemma.

**Lemma 14.** Suppose that $Y_1, \ldots, Y_{2n} \sim N(\beta, I)$. Let $\psi_n(\beta) = P(\sqrt{2n}(\hat{\beta}_S - \beta^*_S) \leq t)$. There is no uniformly consistent estimator of $\psi_n(\beta)$.

**Prediction Accuracy.** Now we discuss prediction accuracy which is where splitting pays a price. The idea is to identify a population quantity $\theta$ that model selection is implicitly targeting and compare splitting versus non-splitting in terms of how well they estimate $\theta$. The purpose of model selection in regression is to choose a model with low prediction error. So, in regression, we might take $\theta$ to be the prediction risk of the best linear model with $k$ terms. In our many-means model, a natural analog of this is the parameter $\theta = \max_j \beta^*_j$.

We have the following lower bound, which applies over all estimators both splitting and non-splitting. For the purposes of this lemma, we use Normality. Of course, the lower bound is even larger if we drop Normality.

**Lemma 15.** Let $Y_1, \ldots, Y_n \sim P$ where $P = N(\beta, I)$, $Y_i \in \mathbb{R}^D$, and $\beta \in \mathbb{R}^D$. Let $\theta = \max_j \beta_j$. Then

$$\inf_{\hat{\theta}} \sup_{\beta} E[(\hat{\theta} - \theta)^2] \geq \frac{2 \log D}{n}.$$  \hspace{1cm} (53)

To understand the implications of this result, let us write

$$\hat{\beta}(S) - \theta = \underbrace{\hat{\beta}(S) - \beta(S)}_{L_1} + \underbrace{\beta(S) - \theta}_{L_2}.$$  \hspace{1cm} (53)

The first term, $L_1$, is the focus of most research on post-selection inference. We have seen it is small for splitting and large for non-splitting. The second term takes into account the variability due to
Figure 1: Horizontal axis: the gap $\beta_{(1)} - \beta_{(2)}$. Blue risk: risk of splitting estimator. Black line: risk of non-splitting estimator.

model selection which is often ignored. Because $L_1$ is of order $n^{-1/2}$ for splitting, and the because the sum is of order $\sqrt{\log D/n}$ it follows that splitting must, at least in some cases, pay a price by have $L_2$ large. In regression, this would correspond to the fact that, in some cases, splitting leads to models with lower predictive accuracy.

Of course, these are just lower bounds. To get more insight, we consider a numerical example. Figure (1) shows a plot of the risk of $\hat{\beta}(\hat{S}) = \hat{Y}(\hat{S})$ for $2n$ (non-splitting) and $n$ (splitting). In this example we see that indeed, the splitting estimator suffers a larger risk. In this example, $D = 1,000$, $n = 50$, and $\beta = (a,0,\ldots,0)$. The horizontal axis is $a$ which is the gap between the largest and second largest mean.

To summarize: splitting gives more precise estimates and coverage for the selected parameter than non-splitting (uniform) inference. But the two approaches can be estimating different parameters. This manifests itself by the fact that splitting can lead to less precise estimates of the population parameter $\theta$. In the regression setting, this would correspond to the fact that splitting the data can lead to selecting models with poorer prediction accuracy.
### 4 Comments on Non-Splitting Methods

There are several methods for constructing confidence intervals in high-dimensional regression. Some approaches are based on debiasing the lasso estimator (e.g., Zhang and Zhang, 2014; van de Geer et al., 2014; Javanmard and Montanari, 2014; Nickl and van de Geer, 2013, See Section 1.1). These approaches tend to require that the linear model to be correct as well as assumptions on the design, and tend to target the true \( \beta \) which is well-defined in this setting. Some partial exceptions exist: Bühlmann and van de Geer (2015) relaxes the requirement of a correctly-specified linear model, while Meinshausen (2015) removes the design assumptions. In general, these debiasing approaches do not provide uniform, assumption-free guarantees.

Lockhart et al. (2014); Lee et al. (2016); Taylor et al. (2014) do not require the linear model to be correct nor do they require design conditions. However, their results only hold for parametric models. Their method works by inverting a pivot.

In fact, inverting a pivot is, in principle, a very general approach. We could even use inversion in the nonparametric framework as follows. For any \( P \in \mathcal{P} \) and any \( j \) define \( t(j,P) \) by

\[
\mathbb{P}(\sqrt{n}|\hat{\beta}_S(j) - \beta_S(j)| > t(j,P)) = \alpha.
\]

Note that, in principle, \( t(j,P) \) is known. For example, we could find \( t(j,P) \) by simulation. Now let \( A = \{ P \in \mathcal{P} : \sqrt{n}|\hat{\beta}_S(j) - \beta_S(j)| < t(j,P) \} \). Then \( \mathbb{P}(P \in A) \geq 1 - \alpha \) for all \( P \in \mathcal{P} \). Write \( \beta_j(S) = f(P, Z_1, \ldots, Z_n) \). Let \( C = \{ f(P, Z_1, \ldots, Z_n) : P \in A \} \). It follows that \( \mathbb{P}(\beta_j(S) \in C) \geq 1 - \alpha \) for all \( P \in \mathcal{P} \). Furthermore, we could also choose \( t(j,P) \) to satisfy \( \mathbb{P}(\sqrt{n}|\hat{\beta}_S(j) - \beta_S(j)| > t(j,P)|E_n) = \alpha \) for any event \( E_n \) which would given conditional confidence intervals if desired.

There are two problems with this approach. First, the confidence sets would be huge. Second, it is not computationally feasible to find \( t(j,P) \) for every \( P \in \mathcal{P} \). The crucial and very clever observation in Lee et al. (2016) is that if we restrict to a parametric model (typically they assume a Normal model with known, constant variance) then, by choosing \( E_n \) carefully, the conditional distribution reduces, by sufficiency, to a simple one parameter family. Thus we only need to find \( t \) for this one parameter family which is feasible. Unfortunately, the method does not provide confidence guarantees of the form (6) which is the goal of this paper.

Berk et al. (2013) is closest to providing the kind of guarantees we have considered here. But as we discussed in the previous section, it does not seem to be extendable to the assumption-free framework.

None of these comments is meant as a criticism of the aforementioned methods. Rather, we just want to clarify that these methods are not comparable to our results because we require uniformity over \( \mathcal{P} \). Also, except for the method of Berk et al. (2013), none of the other methods provide any guarantees over unknown selection rules.
5 Numerical Examples

In this section we briefly consider a few illustrative examples. In a companion paper, we provide detailed simulations comparing all of the recent methods that have proposed for inference after model selection. It would take too much space, and go beyond the scope of the current paper, to include these comparisons here.

We focus on linear models, and in particular on inference for the projected parameter $\hat{\beta}_S$ and the LOCO parameter $\hat{\gamma}_S$ of Section 2.1 and Section 2.2, respectively. The data are drawn from three distributions:

**Setting A** Linear and sparse with Gaussian noise. A linear model with $\beta_i \sim U[0, 1]$ for $j = 1, \ldots, 5$ and $\beta_j = 0$ otherwise.

**Setting B** Additive and sparse with $t$-distributed noise. An additive model with a cubic and a quadratic term, as well as three linear terms, and $t_5$-distributed additive noise.

**Setting C** Non-linear, non-sparse, $t$-distributed noise. The variables from Setting B are rotated randomly to yield a dense model.

In Settings A and B, $n = 100$ (before splitting); in Setting C $n = 200$. In all Settings $p = 50$ and the noise variance is 0.5. The linear model, $\hat{\beta}_S$ is selected on $D_1$ by lasso with $\lambda$ chosen using 10-fold cross-validation. For $\gamma_S(j)$, $\hat{\gamma}_S(j)$ is estimated by reapplying the same selection procedure to $D_1$ with the $j^{th}$ variable removed. Confidence intervals are constructed using the pairs bootstrap procedure of Section 2 with $\alpha = 0.05$.

Figure 2 shows typical confidence intervals for the projection parameter, $\hat{\beta}_S$, and the LOCO parameter, $\hat{\gamma}_S$, for one realization of each Setting. Notice that confidence intervals are only constructed for $j \in \hat{S}$. The non-linear term is successfully covered in Setting B, even though the linear model is wrong.

Figure 3 shows the coverage probability for Setting B as a function of $n$, holding $p = 50$ fixed. The coverage for the LOCO parameter, $\hat{\gamma}_S$ is accurate even at low sample sizes. The coverage for $\hat{\beta}_S$ is low (0.8-0.9) for small sample sizes, but converges to the correct coverage as the sample size grows. This suggests that $\hat{\gamma}_S$ is an easier parameter to estimate and conduct inference on.

6 Berry-Esseen Bounds for Nonlinear Parameters With Increasing Dimension

The results in this paper depend on a Berry-Esseen bound for regression with possibly increasing dimension. In this section, there is no model selection or splitting. We set $d = k$ and $S = \{1, \ldots, k\}$ where $k < n$ and $k$ can increase with $n$. Later, these results will be applied after model selection and sample splitting. Existing Berry-Esseen results for nonlinear parameters are given in Pinelis.
Figure 2: Typical confidence intervals for the projection parameter (left) and the LOCO parameter (right) for Settings A, B, and C. Blue indicates the true parameter value, and green indicates the point estimate from $D_2$. Note that the parameters are successfully covered even when the underlying signal is non-linear ($X_1$ in Setting B) or dense (Setting C).
Figure 3: Joint coverage probability of the intervals for $\beta_S$ and $\gamma_S$ in Setting B, as sample size $n$ varies with $p = 50$ held fixed. The coverage for $\gamma_S$ is accurate even at low sample sizes, while the coverage for $\beta_S$ converges more slowly.

and Molzon (2016); Shao et al. (2016); Chen and Shao (2007); Anastasiou and Reinert (2014); Anastasiou and Ley (2015); Anastasiou and Gaunt (2016). Our results are in the same spirit but we keep careful track of the effect of dimension and the eigenvalues of $\Sigma$, while leveraging results from Chernozhukov et al. (2013, 2014) on high dimensional central limit theorems for simple convex sets.

We derive a general result on the accuracy of the Normal approximation over hyper-rectangles for nonlinear parameters. We make use of three findings from Chernozhukov et al. (2014, 2015) and Nazarov (2003): the Gaussian anti-concentration theorem, the high-dimensional central limit theorem for sparingly convex sets, and the Gaussian comparison theorem, reported in the appendix as Theorems 26, 27 and 28, respectively. In fact, in the appendix we re-state these results in a slightly different form than they appear in the original papers. We do this because we need to keep track of certain constants that affect our results.

Let $W_1, \ldots, W_n$ be an independent sample from a distribution $P$ on $\mathbb{R}^b$ belonging to the class $\mathcal{P}_n$ of probability distribution supported on a subset of $[-A, A]^b$, for some fixed $A > 0$ and such that

$$v = \inf_{P \in \mathcal{P}_n} \lambda_{\min}(V(P)) \quad \text{and} \quad \overline{v} = \sup_{P \in \mathcal{P}_n} \lambda_{\max}(V(P)) \geq 1,$$

where $V(P) = \mathbb{E}_P[(W_i - \psi)(W_i - \psi)^T]$. We allow the class $\mathcal{P}_n$ to change with $n$, so that $b, v$ and $\overline{v}$ but not $A$ are to be regarded as functions of $n$, although we do not express such dependence in our notation for ease of readability. Notice that, in the worse case, $\overline{v}$ can be of order $b$.

**Remark.** The assumption that $\overline{v} \geq 1$ is made out of convenience and is used in the proof of Lemma 24 in the Appendix. Our results remain valid if we assume that $\overline{v}$ is bounded away from 0 uniformly in $n$, i.e. that $\overline{v} \geq \eta$ for some $\eta > 0$ and all $n$. Then, the term $\eta$ would then appear as another quantity affecting the bounds. We have not kept track of this additional dependence.
Let \( g = (g_1, \ldots, g_s)^\top : \mathbb{R}^b \to \mathbb{R}^s \) be a twice-continuously differentiable vector-valued function defined over an open, convex subset \( S_n \) of \([−A, A]^b\) such that, for all \( P \in \mathcal{P}_n \), \( \psi = \psi(P) = E[W] \in S_n \). Let \( \hat{\psi} = \hat{\psi}(P) = \frac{1}{n} \sum_{i=1}^n W_i \) and assume that \( \hat{\psi} \in S_n \) almost surely, for all \( P \in \mathcal{P}_n \). Finally, set \( \theta = g(\hat{\psi}) \) and \( \hat{\theta} = g(\hat{\psi}) \). For any point \( \psi \in S_n \) and \( j \in \{1, \ldots, s\} \), we will write \( G_j(\psi) \in \mathbb{R}^b \) and \( H_j(\psi) \in \mathbb{R}^{b \times b} \) for the gradient and Hessian of \( g_j \) at \( \psi \), respectively. We will set \( G(\psi) \) to be the \( s \times b \) Jacobian matrix whose \( j \)th row is \( G_j(\psi) \).

**Remark.** The assumption that \( \hat{\psi} \) belongs to \( S_n \) almost surely can be relaxed to hold on an event of high probability, resulting in an additional error term in all our bounds.

To derive a high-dimensional Berry-Esseen bound on \( g(\psi) - g(\hat{\psi}) \) we will study its first order Taylor approximation. Towards that end, we will require a uniform control over the size of the gradient and Hessian of \( g \). Thus we set

\[
B = \sup_{P \in \mathcal{P}_n} \max_{j=1,\ldots,s} ||G_j(\psi(P))|| \quad \text{and} \quad \overline{H} = \sup_{\psi \in S_n} \max_{j=1,\ldots,s} ||H_j(\psi)||_{\text{op}}
\]

where \( ||H_j(\psi)||_{\text{op}} \) is the operator norm.

**Remark.** The quantity \( \overline{H} \) can be defined differently, as a function of \( \mathcal{P}_n \) and not \( S_n \). In fact, all that is required of \( \overline{H} \) is that it satisfy the almost everywhere bound

\[
\max_j \int_0^1 \left\| H_j \left( t\psi(P) - (1-t)\hat{\psi}(P) \right) \right\|_{\text{op}} dt \leq \overline{H},
\]

for each \( P \in \mathcal{P}_n \) (see (88) below). This allows us to establish a uniform bound on the magnitude of the reminder term in the Taylor series expansion of \( g(\hat{\psi}) \) around \( g(\psi) \), as detailed in the proof of Theorem 16 below. Of course, we may relax the requirement that (55) holds almost everywhere to the requirement that it holds on an event of high probability. This is indeed the strategy we use when in applying the present results to the projection parameters in Section 2.1.

The covariance matrix of the linear approximation of \( g(\psi) - g(\hat{\psi}) \), which, for any \( P \in \mathcal{P}_n \), is given by

\[
\Gamma = \Gamma(\psi(P), P) = G(\psi(P))V(P)G(\psi(P))^\top,
\]

plays a crucial role in our analysis. In particular, our results will depend on the smallest variance of the linear approximation to \( g(\psi) - g(\hat{\psi}) \):

\[
\sigma^2 = \inf_{P \in \mathcal{P}_n} \min_{j=1,\ldots,s} G_j(\psi(P))V(P)G_j(\psi(P)).
\]

With these definitions in place we are now ready to prove the following high-dimensional Berry-Esseen bound.

**Theorem 16.** Assume that \( W_1, \ldots, W_n \) is an i.i.d. sample from some \( P \in \mathcal{P}_n \) and let \( Z_n \sim N(0, \Gamma) \). Then, there exists a \( C > 0 \), dependent on \( A \) only, such that

\[
\sup_{P \in \mathcal{P}_n} \sup_{t > 0} \left| \mathbb{P}(\sqrt{n}||\theta - \hat{\theta}||_\infty \leq t) - \mathbb{P}(||Z_n||_\infty \leq t) \right| \leq C \left( \Delta_{n,1} + \Delta_{n,2} \right),
\]

(58)

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where

\[ \Delta_{n,1} = \frac{1}{\sqrt{v}} \left( \frac{v^2 b (\log 2bn)^7}{n} \right)^{1/6} \] (59)

\[ \Delta_{n,2} = \frac{1}{\sigma} \frac{1}{\sqrt{n}} \left( \frac{b^2 \log b}{n} \right)^{1/6} \] (60)

**Remarks** The assumption that the support of \( P \) is compact is made for simplicity, and can be modified by assuming that the coordinates of the vectors \( W_i \) have sub-exponential behavior. Notice also that the coordinates of the \( W_i \)'s need not be independent.

The proof of Theorem 16 resembles the classic proof of the asymptotic normality of non-linear functions of averages by the delta method. First, we carry out a coordinate-wise Taylor expansion of \( \hat{\theta} \) around \( \theta \). We then utilize a a high-dimensional Berry-Esseen theorem for polyhedral sets established in Chernozhukov et al. (2014) (see Lemma 24 below for details) to derive a Gaussian approximation to the linear part in the expansion, resulting in the error term \( \Delta_{n,1} \). Finally, we bound the reminder term due to the non-linearity of the function \( g \) with basic concentration arguments paired with the Gaussian anti-concentration bound due to Nazarov (2003) (see Theorem 26 in the Appendix), thus obtaining the second error term \( \Delta_{n,2} \). Throughout, we keep track of the dependence on \( v \) and \( \sigma \) in order to obtain rates with a leading constant dependent only on \( A \) (assumed fixed) but not on any other term that may vary with \( k \) or \( b \).

**Asymptotically honest confidence sets: Normal approximation approach**

We now show how to use the high-dimensional central limit theorem Theorem 16 to construct asymptotically honest confidence sets for \( \theta \). We will first to obtain a consistent estimator of the covariance matrix \( \Gamma = G(\psi)V(\psi)G(\psi)^\top \) of the linear approximation to \( \hat{\theta} - \theta \). In conventional fixed-dimension asymptotics, we would appeal to Slutsky’s theorem and ignore the effect of replacing \( \Gamma \) with a consistent estimate. But in computing Berry-Esseen bounds with increasing dimension we may not discard the effect of estimating \( \Gamma \). As we will see below, this extra step will bring an additional error term that must be accounted for. We will estimate \( \Gamma \) with the plug-in estimator

\[ \hat{\Gamma} = G(\hat{\psi})\hat{V}G(\hat{\psi})^\top, \] (61)

where \( \hat{\psi} = \frac{1}{n} \sum_{i=1}^{n} W_i W_i^\top \) is the empirical covariance matrix. Below, we bound the element-wise difference between \( \Gamma \) and \( \hat{\Gamma} \). Although this is in general a fairly weak notion of consistency in covariance matrix estimation, it is all that is needed to apply the Gaussian comparison theorem 28, which will allow us to extend the Berry-Esseen bound established in Theorem 16 to the case when \( \Gamma \) is estimated.

**Lemma 17.** Let

\[ \kappa_n = \max \left\{ HB\sqrt{\frac{b\log n}{n}}, B^2 \sqrt{b\sigma b + \log n} \right\}. \] (62)

There exists a \( C > 0 \) dependent on \( A \) only such that

\[ \sup_{P \in \mathcal{P}_n} \mathbb{P} \left( \max_{j,l} \left| \hat{\Gamma}(j,l) - \Gamma(j,l) \right| \geq C \kappa_n \right) \leq \frac{2}{n}. \] (63)
Now we construct the confidence set. Let \( Q = (Q(1), \ldots, Q(s)) \) be i.i.d. standard Normal variables, independent of the data. Let \( \tilde{Z} = \tilde{\Gamma}^{1/2}Q \) and define \( \tilde{t}_\alpha \) by
\[
\mathbb{P}(||\tilde{Z}||_\infty > \tilde{t}_\alpha | \tilde{\Gamma}) = \alpha.
\] (64)

Finally, let
\[
\tilde{C}_n = \{ \theta \in \mathbb{R}^s : ||\theta - \tilde{\theta}||_\infty \leq \frac{\tilde{t}_\alpha}{\sqrt{n}} \}.
\] (65)

**Theorem 18.** There exists a \( C > 0 \), dependent only on \( A \), such that
\[
\inf_{P \in \mathcal{P}} \mathbb{P}(\theta \in R_n) = 1 - \alpha - C \left( \Delta_{n,1} + \Delta_{n,2} + \Delta_{n,3} + \frac{1}{n} \right),
\] (66)
where
\[
\Delta_{n,3} = \frac{8n^{1/3}(2 \log 2s)^{2/3}}{\sigma^{2/3}}.
\] (67)

**Remark.** The additional term \( \Delta_{n,3} \) in the previous theorem is due to the uncertainty in estimating \( \Gamma \), and can be established by using the comparison inequality for Gaussian vectors of Chernozhukov et al. (2015), keeping track of the dependence on \( \sigma^2 \); see Theorem 28 below.

In addition to \( L_\infty \) balls, we can also construct our confidence set to be a hyper-rectangle, with side lengths proportional to the standard errors of the projection parameters. That is, we define
\[
\tilde{C}_n = \bigotimes_{j \in S} C(j),
\] (68)
where
\[
C(j) = \left[ \hat{\beta}_S(j) - z_{\alpha/(2s)} \sqrt{\tilde{\Gamma}_n(j,j) / n}, \hat{\beta}_S(j) + z_{\alpha/(2s)} \sqrt{\tilde{\Gamma}_n(j,j) / n} \right],
\] with \( \tilde{\Gamma} \) given by (16) and \( z_{\alpha/(2s)} \) the upper \( 1 - \alpha/(2s) \) quantile of a standard normal variate. Notice that we use a Bonferroni correction to guarantee a nominal coverage of \( 1 - \alpha \). Also, note that \( z_{\alpha/(2s)} = O(\sqrt{\log s}) \), for each fixed \( \alpha \). The coverage rate for this other confidence set is derived in the next result.

**Theorem 19.** Let
\[
\tilde{\Delta}_{n,3} = \min \left\{ \Delta_{n,3}, \frac{\mathbb{E}_n z_{\alpha/(2s)}}{\sigma^2} \left( \sqrt{2 + \log(2s)} + 2 \right) \right\}.
\] (69)
There exists a \( C > 0 \), dependent only on \( A \), such that
\[
\inf_{P \in \mathcal{P}_n} \mathbb{P}(\theta \in \tilde{C}_n) \geq (1 - \alpha) - C (\Delta_{n,1} + \Delta_{n,2} + \tilde{\Delta}_{n,3} + \frac{1}{n}).
\]
Asymptotically honest confidence sets: the bootstrap approach

To construct the confidence set (65), one has to compute the estimator \( \hat{\Gamma} \) and the quantile \( \hat{t}_\alpha \) in (64), which may be computationally inconvenient. Similarly, the hyper-rectangle (68) requires computing the diagonal entries in \( \hat{\Gamma} \).

Below we rely on the bootstrap to construct analogous confidence sets, centered at \( \hat{\theta} \), which do not need knowledge of \( \hat{\Gamma} \). We let \( \hat{\psi}_* \) denote the sample average of an i.i.d. sample of size \( n \) from the bootstrap distribution, which is the empirical measure associated to the sample \( (W_1,\ldots,W_n) \). We also let \( \hat{\theta}_* = g(\hat{\psi}_*) \).

For a fixed \( \alpha \in (0,1) \), let \( \hat{t}_* \) be the smallest positive number such that

\[
\mathbb{P} \left( \sqrt{n} \| \hat{\theta} - \hat{\theta} \| \leq \hat{t}_* \bigg| (W_1,\ldots,W_n) \right) \geq 1 - \alpha.
\]

and let \( (\hat{t}_j^*, j = 1,\ldots,s) \) be such that

\[
\mathbb{P} \left( \sqrt{n} | \hat{\theta}_*(j) - \hat{\theta}(j) | \leq \hat{t}_j^*, \forall j \bigg| (W_1,\ldots,W_n) \right) \geq 1 - \alpha.
\]

By the union bound, each \( \hat{t}_j^* \) can be chosen to be the largest positive number such that

\[
\mathbb{P} \left( \sqrt{n} | \hat{\theta}_*(j) - \hat{\beta}(j) | > \hat{t}_j^*, \bigg| (W_1,\ldots,W_n) \right) \leq \frac{\alpha}{s}.
\]

Consider the following two bootstrap confidence sets:

\[
\hat{C}_n^* = \left\{ \theta \in \mathbb{R}^s : \| \theta - \hat{\theta} \|_{\infty} \leq \frac{\hat{t}_*}{\sqrt{n}} \right\} \quad \text{and} \quad \tilde{C}_n^* = \left\{ \theta \in \mathbb{R}^s : | \theta(j) - \hat{\theta}(j) | \leq \frac{\tilde{t}_j^*}{\sqrt{n}}, \forall j \in \hat{S} \right\}
\]

(70)

**Theorem 20.** Assume the same conditions of Theorem 16 and that and \( \hat{\psi} \) and \( \hat{\psi}_* \) belong to \( S_n \) almost surely. Suppose that \( n \) is large enough so that the quantities \( \sigma_n^2 = \sigma^2 - C \kappa_n > 0 \) and \( v_n = \nu - C \gamma_n \) are positive, where \( C \) is the larger of the two constants in (63) and in (104) and

\[
\gamma_n = \sqrt{b \frac{\log b + \log n}{n}}.
\]

Also set \( \nu_n = \nu + C \gamma_n \). Then, for a constant \( C \) depending only on \( A \),

\[
\inf_{P \in \mathcal{P}_n} \mathbb{P}(\theta \in \hat{C}_n^* \cap \tilde{C}_n^*) \geq 1 - \alpha - C \left( \Delta_{n,1}^* + \Delta_{n,2}^* + \Delta_{n,3}^* + \frac{1}{n} \right),
\]

(71)

where

\[
\Delta_{n,1}^* = \frac{1}{\sqrt{v_n}} \left( \frac{\nu_n b (\log 2bn)^2}{n} \right)^{1/6}, \quad \Delta_{n,2}^* = \frac{1}{\sigma_n} \sqrt{b \nu_n \hat{\theta}^2 \log n \log b},
\]

and \( \Delta_{n,3}^* \) is given in (67). Similarly,

\[
\inf_{P \in \mathcal{P}_n} \mathbb{P}(\theta \in \hat{C}_n^* \cap \tilde{C}_n^*) \geq 1 - \alpha - C \left( \Delta_{n,1}^* + \Delta_{n,2}^* + \Delta_{n,3}^* + \frac{1}{n} \right).
\]

(72)
Remark. The assumption that $\hat{\psi}$ and $\hat{\psi}^*$ are in $S_n$ almost surely can be relaxed to a high probability statement without any issue, resulting in an additional bound on the probability of the complementary event.

Remark. The proof of the theorem involves enlarging the class of distributions $P_n$ to a bigger collection $P_n^*$ that is guaranteed to include the bootstrap distribution (almost surely or with high probability). The resulting coverage error terms are larger than the ones obtained in Theorem 18 using Normal approximations precisely because $P_n^*$ is a larger class. In the above result we simply increase the rates arising from Theorem 18 so that they hold for $P_n^*$ without actually recomputing the quantities $B$, $H$ and $\sigma^2$ in (54) and (57) over the new class $P_n^*$. Of course, better rates may be established should sharper bounds on those quantities be available.

Remark. The error term $\Delta_{n,3}$ remains the same as in Theorem 18 and Theorem 19 because it quantifies an error term, related to the Gaussian comparison Theorem 28, which does not depend on the bootstrap distribution.

7 Conclusions

In this paper we have taken a modern look at inference based on sample splitting. We have also investigated the accuracy of Normal and bootstrap approximations and we have suggested new parameters for regression.

Despite the fact that sample splitting is on old idea, there remain many open questions. For example, in this paper, we focused on a single split of the data. One could split the data many times and somehow combine the confidence sets. However, for each split we are essentially estimating a different (random) parameter. So currently, it is nor clear how to combine this information.

The bounds on coverage accuracy — which are of interest beyond sample splitting — are upper bounds. An important open question is to find lower bounds. Also, it is an open question whether we can improve the bootstrap rates. For example, the remainder term in the Taylor approximation of $\sqrt{n}(\hat{\beta}(j) - \beta(j))$ is

$$\frac{1}{2n} \int \int \delta^\top H_j((1 - t)\psi + t\hat{\psi})\delta \, dt$$

where $\delta = \sqrt{n}(\hat{\psi} - \psi)$. By approximating this quadratic term it might be possible to correct the bootstrap distribution. Pouzo et al. (2015) has results for bootstrapping quadratic forms that could be useful here. In Section 8 we saw that a modified bootstrap, that we called the image bootstrap, has very good coverage accuracy even in high dimensions. Future work is needed to compute the resulting confidence set efficiently.

Finally, we remind the reader that we have taken a assumption-free perspective. If there are reasons to believe in some parametric model then of course the distribution-free, sample splitting approach used in this paper will be sub-optimal.
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8 Appendix 1: Improving the Coverage Accuracy of the Bootstrap for the Projection Parameters

Throughout, we treat $S$ as a fixed, non-empty subset of $\{1, \ldots, d\}$ of size $k$ and assume an i.i.d. sample $(Z_1, \ldots, Z_n)$ where $Z_i = (X_i, Y_i)$ for all $i$, from a distribution from $\mathcal{P}_n^{\text{OLS}}$.

The coverage accuracy for LOCO and prediction parameters is much higher than for the projection parameters and the inferences for $\beta_S$ are less accurate if $k$ is allowed to increase with $n$. Of course, one way to ensure accurate inferences is simply to focus on $\gamma_S$ or $\phi_S$ instead of $\beta_S$. Here we discuss some other approaches to ensure coverage accuracy.

If we use ridge regression instead of least squares, the gradient and Hessian with respect to $\beta$ are bounded and the error terms are very small. However, this could degrade prediction accuracy. This leads to a tradeoff between inferential accuracy and prediction accuracy. Investigating this tradeoff will be left to future work.

Some authors have suggested the estimator $\hat{\beta}_S = \tilde{\Sigma}_S^{-1} \tilde{\alpha}_S$ where $\tilde{\Sigma}_S$ is a block diagonal estimator of $\Sigma$. If we restrict the block size to be bounded above by a constant, then we get back the accuracy of the sparse regime. Again there is a tradeoff between inferential accuracy and prediction accuracy.

The accuracy of the bootstrap can be increased by using the image bootstrap as we now describe. First we apply the bootstrap to get a confidence set for $\psi_S$. Let

$$H_n = \left\{ \psi_S : ||\psi_S - \hat{\psi}_S||_{\infty} \leq \frac{t^*_a}{\sqrt{n}} \right\}$$

where $t^*_a$ is the bootstrap quantile defined by $\hat{F}^*(t^*_a) = 1 - \alpha$ and $\hat{F}^*(t) = P(\sqrt{n}||\hat{\psi}_S^* - \hat{\psi}_S||_{\infty} \leq t | Z_1, \ldots, Z_n)$.

Since $\psi_S$ is just a vector of moments, it follows from Theorem 27 Theorem K.1 of Chernozhukov et al. (2013) and the Gaussian anti-concentration (Theorem 26) that, for a constant $C$ depending on $A$ only,

$$\sup_{P \in \mathcal{P}_n^{\text{OLS}}} |P(\psi \in H_n) - (1 - \alpha)| \leq \frac{C}{a_n} \left( \frac{(\log k)^7}{n} \right)^{1/6}.$$

In the above display $a_n = \sqrt{a - C \sqrt{\frac{\log k}{n}}}$ and is positive for $n$ large enough, and

$$a \leq \inf_{P \in \mathcal{P}_n^{\text{OLS}}} \min_{j \in \{1, \ldots, d\}} \text{Var}_P(W_i(j)).$$

Notice that $a$ is positive since $a \geq v$, where $v$ is given the definition 1 of $\mathcal{P}_n^{\text{OLS}}$. However, $a$ can be significantly larger than $v$. The term $C \sqrt{\log kn}$ appearing in the definition of $a_n$ is just a high probability bound on the maximal element-wise difference between $V$ and $\hat{V}$, valid for each $P \in \mathcal{P}_n^{\text{OLS}}$. 43
Next, recall that $\beta_S = g(\psi_S)$. Now define

$$C_n = \left\{ g(\psi) : \psi \in H_n \right\}. \tag{74}$$

We call $C_n$ the *image bootstrap confidence set* as it is just the nonlinear function $g$ applied to the confidence set $H_n$. Then, by (73),

$$\inf_{P \in P_n} \mathbb{P}(\beta \in C_n) \geq 1 - \alpha - \frac{C}{a_n} \left( \frac{\log k}{n} \right)^{1/6}. \tag{75}$$

In particular, the implied confidence set for $\beta(j)$ is

$$C_j = \left[ \inf_{\psi \in H_n} g(\psi), \sup_{\psi \in H_n} g(\psi) \right].$$

Remarkably, in the coverage accuracy of the image-bootstrap the dimension $k$ enters only logarithmically. This is in stark contrast with the coverage accuracy guarantees for the projection parameters from Section 2.1, which depend polynomially in $k$ and on the other eigenvalue parameters.

The image bootstrap is usually avoided because it generally leads to conservative confidence sets. Below we derive bounds on the accuracy of the image bootstrap.

**Theorem 21.** Let $u_n$ be as in (20) and assume that $k \geq u_n^2$. Then, for each $P \in P_n^{\text{OLS}}$, with probability at least $1 - \alpha$, the diameter of the image bootstrap confidence set $H_n$ is bounded by

$$C \frac{k^{3/2}}{u_n^2} \sqrt{\frac{\log k + \log n}{n}}.$$

where $C > 0$ depends on $A$ only.

**Remark.** The assumption that $k \geq u_n^2$ is not necessary and can be relaxed, resulting in a slightly more general bound.

Assuming non-vanishing $u$, the diameter tends uniformly to 0 if $k(\log k)^{1/3} = o(n^{1/3})$. Interestingly, this is the same condition required in Portnoy (1987) although the setting is quite different.

Currently, we do not have a computationally efficient method to find the supremum and infimum. A crude approximation is given by taking a random sample $\psi_1, \ldots, \psi_N$ from $H_n$ and taking

$$a(j) \approx \min_j g(\hat{\psi}_j), \quad b(j) \approx \max_j g(\hat{\psi}_j).$$

**Proof of Theorem 21.** We will establish the claims by bound the quantity $\|\hat{\beta}_S - \beta_S\|$ uniformly over all $\beta_S \in H_n$. Our proof relies on a first order Taylor series expansion of $g$ and on the uniform bound on the norm of the gradient of each $g_j$ given in (78). Recall that, by conditioning on $D_{1,n}$, we can regard $S$
and \(\beta_S\) as a fixed. Then, letting \(G(x)\) be the \(|S| \times b\)-dimensional Jacobian of \(g\) at \(x\) and using the mean value theorem, we have that

\[
\|\hat{\beta}_S - \beta_S\| = \left\| \left( \int_0^1 G((1-t)\psi_S + ut\hat{\psi}_S)dt \right) (\hat{\psi}_S - \psi_S) \right\| \\
\leq \left\| \int_0^1 G((1-t)\psi_S + t\hat{\psi}_S)dt \right\|_{op} \|\hat{\psi}_S - \psi_S\|.
\]

To further bound the previous expression we use the fact, established in the proof of Lemma 17, that \(\|\hat{\psi}_S - \psi_S\| \leq Ck \sqrt{\frac{\log n + \log k}{n}}\) with probability at least \(1/n\), where \(C\) depends on \(A\), for each \(P \in P_n^{\text{OLS}}\). Next,

\[
\left\| \int_0^1 G((1-t)\psi_S + t\hat{\psi}_S)dt \right\|_{op} \leq \sup_{t \in (0,1)} \left\| G \left( (1-t)\psi_S + t\hat{\psi}_S \right) \right\|_{op} \leq \sup_{t \in (0,1)} \max_{j \in S} \left\| G \left( (1-t)\psi_S + t\hat{\psi}_S \right) \right\|
\]

where \(G_j(\psi)\) is the \(j\)th row of \(G(\psi)\), which is the gradient of \(g_j\) at \(\psi\). Above, the first inequality relies on the convexity of the operator norm and the second inequality uses that the fact that the operator norm of a matrix is bounded by the maximal Euclidean norm of the rows. For each \(P \in P_n^{\text{OLS}}\) and each \(t \in (0,1)\) and \(j \in S\), the bound in (113) yields that, for a \(C > 0\) depending on \(A\) only,

\[
\left\| G \left( (1-t)\psi_S + t\hat{\psi}_S \right) \right\| \leq C \left( \frac{\sqrt{k}}{u_t^2} + \frac{1}{u_t} \right),
\]

where \(\hat{u}_t \geq (1-t)\lambda_{\min}(\Sigma_S) + t\lambda_{\min}(\hat{\Sigma}_S)\). By (104) in Lemma 25 and Weyl’s theorem, and using the fact that \(u > u_n\), on an event with probability at least \(1 - \frac{1}{n}\),

\[
\left\| G \left( (1-t)\psi_S + t\hat{\psi}_S \right) \right\| \leq C \left( \frac{\sqrt{k}}{u_n^2} + \frac{1}{u_n} \right) \leq C \frac{\sqrt{k}}{u_n^2},
\]

where in the last inequality we assume \(n\) large enough so that \(k \geq u_n^2\). The previous bound does not depend on \(t, j\) or \(P\). The result now follows. \(\square\)

9  Appendix 2: Proofs of the results in Section 2

In all the proofs of the results from Section 2, we will condition on the outcome of the sample splitting step, resulting in the random equipartition \(I_{1,n}\) and \(I_{2,n}\) of \(\{1, \ldots, 2n\}\), and on \(D_{1,n}\). Thus, we can treat the outcome of the model selection and estimation procedure \(w_n\) on \(D_{1,n}\) as a fixed. As a result, we regard \(\hat{S}\) as a deterministic, non-empty subset of \(\{1, \ldots, d\}\) of size by \(k < d\) and the projection parameter \(\hat{\beta}_S\) as a fixed vector of length \(k\). Similarly, for the LOCO parameter \(\gamma_{\hat{S}}\), the quantities \(\hat{\beta}_{S}\) and \(\hat{\beta}_{S(j)}\), for \(j \in \hat{S}\), which depend on \(D_{1,n}\) also become fixed. Due to the independence of \(D_{1,n}\) and \(D_{2,n}\), all the probabilistic statements made in the proofs are therefore referring to the randomness in \(D_{2,n}\) only. Since all our bounds will depend on \(D_{1,n}\) through the cardinality of \(\hat{S}\), which is fixed at \(k\), the same bounds will hold uniformly over all possible values
taken on by $D_{1,n}$ and $I_{1,n}$ and all possible outcomes of all model selection and estimation procedures $w_n \in \mathcal{W}_n$ run on $D_{1,n}$. In particular, the bounds are valid unconditionally with respect to the joint distribution of the entire sample and of the splitting outcome.

Also, in the proof $C$ denotes a positive positive that may depend on $A$ only but not on any other variable, and whose value may change from line to line.

**Proof of Theorem 1.** As usual, we condition on $D_{1,n}$ and thus treat $\hat{S}$ as a fixed subset of $\{1, \ldots, d\}$ of size $k$. Recalling the definitions of $\hat{\beta}_{\hat{S}}$ and $\beta_{\hat{S}}$ given in (10) and (1), respectively, and dropping the dependence on $\hat{S}$ in the notation for convenience, we have that

$$\|\hat{\beta}_{\hat{S}} - \beta_{\hat{S}}\| = \|\left(\hat{\Sigma}^{-1} - \Sigma^{-1}\right) \hat{\alpha} + \Sigma^{-1} (\tilde{\alpha} - \alpha)\|$$

$$\leq \|\hat{\Sigma}^{-1} - \Sigma^{-1}\|_{op} \|\hat{\alpha}\| + \frac{1}{u} \|\tilde{\alpha} - \alpha\|$$

$$= T_1 + T_2.$$

By the vector Bernstein inequality (103),

$$\|\tilde{\alpha} - \alpha\| \leq C A \sqrt{\frac{k \log n}{n}},$$

with probability at least $1 - \frac{1}{n}$ and for some universal constant $C$ (independent of $A$). Since the smallest eigenvalue of $\Sigma$ is bounded from below by $u$, we have that

$$T_1 \leq C \frac{1}{u} \sqrt{\frac{k \log n}{n}}.$$

To bound $\|\hat{\Sigma}^{-1} - \Sigma^{-1}\|_{op}$ in the term $T_2$ we write $\hat{\Sigma} = \Sigma + E$ and assume for the moment that $\|E\|_{op} \|\Sigma^{-1}\|_{op} < 1$ (which of course implies that $\|E\Sigma^{-1}\|_{op} < 1$). Since $E$ is symmetric, we have, by formula 5.8.2 in Horn and Johnson (2012), that

$$\|\hat{\Sigma}^{-1} - \Sigma^{-1}\|_{op} = \|(\Sigma + E)^{-1} - \Sigma^{-1}\|_{op} \leq \|\Sigma^{-1}\|_{op} \frac{\|E\Sigma^{-1}\|_{op}}{1 - \|E\Sigma^{-1}\|_{op}},$$

which in turn is upper bounded by

$$\|\Sigma^{-1}\|_{op}^2 \frac{\|\hat{\Sigma} - \Sigma\|_{op}}{1 - \|\hat{\Sigma} - \Sigma\|_{op} \|\Sigma^{-1}\|_{op}}.$$

The matrix Bernstein inequality (104) along with the assumption that $U \geq \eta > 0$ yield that, for a positive $C$ (which depends on $\eta$),

$$\|\hat{\Sigma} - \Sigma\|_{op} \leq C A \sqrt{k U \log k + \log n},$$

with probability at least $1 - \frac{1}{n}$. Using the fact that $\|\Sigma^{-1}\|_{op} \leq \frac{1}{u}$ and the assumed asymptotic scaling on $B_n$ we see that $\|\Sigma^{-1} E\|_{op} \leq 1/2$ for all $n$ large enough. Thus, for all such $n$, we obtain that, with probability at least $1 - \frac{1}{n}$,

$$T_2 \leq 2 CA \frac{k}{u^2} \sqrt{U \log k + \log n},$$

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since \( \|\hat{\alpha}\| \leq A\sqrt{k} \) almost surely. Thus we have shown that (15) holds, with probability at least \( 1 - \frac{2}{n} \) and for all \( n \) large enough. This bound holds uniformly over all \( P \in \mathcal{P}_n^{\text{OLS}} \). \( \square \)

**Proof of Theorem 2.** In what follows, any term of the order \( \frac{1}{n} \) are absorbed into terms of asymptotic bigger order.

As remarked at the beginning of this section, we first condition on \( \mathcal{D}_{1,n} \) and the outcome of the sample splitting, so that \( \hat{S} \) is regarded as a fixed non-empty subset \( S \) of \( \{1, \ldots, d\} \) of size at most \( k \). The bounds (21) and (22) are established using Theorem 18 and Theorem 19 from Section 6, where we may take the function \( g \) as in (14), \( s = k \), \( b = \frac{k^2 + 3k}{2} \) and \( \psi = \psi_S \) and \( \hat{\psi}_S \) as in (12) and (13), respectively. As already noted, \( \psi \) is always in the domain of \( g \) and, as long as \( n \geq d \), is so is \( \hat{\psi} \), almost surely. A main technical difficulty in applying the results of Section 6 is to obtain good approximations for the quantities \( \sigma, \overline{\Sigma} \) and \( B \). This can be accomplished using the bounds provided in Lemma 22 below, which rely on matrix-calculus. Even so, the claims in the theorem do not simply follow by plugging those bounds in Equations (59), (67) and (69) from Section 6. Indeed, close inspection of the proof of Theorem 16 (which is needed by both Theorems 18 and 19) shows that the quantity \( \overline{\Sigma} \), defined in (54), is used there only once, but critically, to obtain the almost everywhere bound in Equation (88). Adapted to the present setting, such a bound would be of the form

\[
\max_{j \in S} \int_0^1 \left\| H_j \left( (1-t)\psi_S(P) + t\hat{\psi}_S(P) \right) \right\|_{\text{op}} \, dt \leq \overline{\Sigma},
\]

almost everywhere, for each \( S \) and \( P \in \mathcal{P}_n^{\text{OLS}} \), where \( \psi_S = \psi_S(P) \) and \( \hat{\psi}_S = \hat{\psi}(P) \) are given in (12) and (13), respectively. Unfortunately, the above inequality cannot be expected to hold almost everywhere, like we did in Section 6. Instead we will derive a high probability bound. In detail, using the second inequality in (78) below we obtain that, for any \( t \in [0, 1] \), \( S, j \in S \) and \( P \in \mathcal{P}_n^{\text{OLS}} \),

\[
\left\| H_j \left( (1-t)\psi_S(P) + t\hat{\psi}_S(P) \right) \right\|_{\text{op}} \leq \frac{C k}{u_n^3},
\]

where \( \hat{u}_t = \lambda_{\text{min}}(t\Sigma_S + (1-t)\hat{\Sigma}_S) \geq t\lambda_{\text{min}}(\Sigma_S) + (1-t)\lambda_{\text{min}}(\hat{\Sigma}_S) \) and the constant \( C \) is the same as in (78) (the dependence \( \Sigma_S \) and \( \hat{\Sigma}_S \) on \( P \) is implicit in our notation). Notice that, unlike in (54) in the proof of Theorem 16, the above bound is random. By assumption, \( \lambda_{\text{min}}(\Sigma_S) \geq u \) and, by (104) in Lemma 25 and Weyl’s theorem, \( \lambda_{\text{min}}(\hat{\Sigma}_S) \geq u \) with probability at least \( 1 - \frac{1}{n} \) for each \( P \in \mathcal{P}_n \).

Since \( u_n \leq u \), we conclude that, for each \( S, j \in S \) and \( P \in \mathcal{P}_n^{\text{OLS}} \),

\[
\max_{j \in S} \int_0^1 \left\| H_j \left( (1-t)\psi_S(P) + t\hat{\psi}_S(P) \right) \right\|_{\text{op}} \, dt \leq \frac{C k}{u_n^3},
\]

on an event of probability at least \( 1 - \frac{1}{n} \). The same arguments apply to the bound (95) in the proof Lemma 17, yielding that the term \( \kappa_n \), given in (62), can be bounded, on an event of probability at least \( 1 - \frac{1}{n} \) and using again Lemma 22, by

\[
C \frac{k^{5/2}}{u_n^3 u^2} \sqrt{\log n},
\]

for each \( P \in \mathcal{P}_n^{\text{OLS}} \) and some \( C > 0 \) dependent on \( A \) only. (In light of the bounds derived next in Lemma 22, the dominant term in the bound on \( \kappa_n \) given in (63) is \( \overline{\Sigma} B \sqrt{\sqrt{b \log n}} \), from which (75) follows. We omit the details).
Thus, for each \( p_0 \in P_{n}^{\text{OLS}} \), we may now apply Theorems 18 and 19 on event with probability no smaller than \( 1 - \frac{1}{n} \), whereby the term \( \overline{P} \) is replaced by \( C \frac{k}{u^2} \) and the terms \( B \) and \( \overline{\sigma} \) are bounded as in Lemma 22.

**Lemma 22.** For any \( j \in \hat{S} \), let \( \beta_{\hat{S}}(j) = e_j^\top \beta_{\hat{S}} = g_j(\psi) \) where \( e_j \) is the \( j^{\text{th}} \) standard unit vector. Write \( \alpha = \alpha_{\hat{S}} \) and \( \Omega = \Sigma_{\hat{S}}^{-1} \) and assume that \( k \geq u^2 \). The gradient and Hessian of \( g_j \) are given by

\[
G_j^\top = e_j \left( \left[ -\left( \alpha^\top \otimes I_k \right) \left( \Omega \otimes \Omega \right) \right] \right) D_h \tag{76}
\]

and

\[
H_j = D_h^\top A_j D_h, \tag{77}
\]

respectively, where

\[
A_j = \frac{1}{2} \left( (I_b \otimes e_j^\top) H + H^\top (I_b \otimes e_j) \right),
\]

and \( D_h \) is the modified duplication matrix defined by \( D_{\psi} = \psi \), with \( \psi \) the vector consisting of the subset of \( \psi \) not including entries that correspond to the upper diagonal entries of \( \Sigma \). Assume that \( k \geq u^2 \). Then,

\[
B = \sup_{p_0 \in P_n^{\text{OLS}}} \max_j \|G_j(p)\| \leq \frac{C \sqrt{k}}{u^2}, \quad \overline{P} = \max_j \sup_{p_0 \in P_n^{\text{OLS}}} \|H_j(p)\|_{\text{op}} \leq \frac{C k}{u^2}, \tag{78}
\]

and

\[
\underline{\sigma} = \inf_{p_0 \in P_n^{\text{OLS}}} \min_j \sqrt{G_j V G_j^\top} \geq \frac{\sqrt{u}}{U}, \tag{79}
\]

where \( C > 0 \) depends on \( A \) only.

**Remark.** The assumption that \( k \geq u^2 \) is not actually needed but this is the most common case and it simplifies the expressions a bit.

**Proof of Corollary 3.** The maximal length is of the sides of \( \tilde{C}_n \) is

\[
2 \max_{j \in \hat{S}} z_{\alpha/(2k)} \sqrt{\frac{\hat{S}(j,j)}{n}} \leq 2 \max_{j \in \hat{S}} z_{\alpha/(2k)} \sqrt{\frac{\Gamma_{\hat{S}}(j,j) + \hat{\Gamma}(j,j) - \Gamma(j,j)}{n}}.
\]

By Lemma 17 and Equation (75), the event that

\[
\max_{j,l \in \hat{S}} \left| \hat{\Gamma}(j,l) - \Gamma(j,l) \right| \leq C \frac{k^{3/2}}{u_n^2 u^2} \sqrt{\frac{k^2 \log n}{n}}
\]

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holds with probability at least $1 - \frac{2}{n}$ and for each $P \in \mathcal{P}^{\text{OLS}}_n$, where $C > 0$ depends on $A$ only. Next, letting $G = G(\hat{s})$ and $V = V_{\hat{s}}$, we have that, for each $j \in \hat{s}$ and $P \in \mathcal{P}^{\text{OLS}}_n$,

$$
\Gamma_{\hat{s}}(j,j) = G_j V G_j^\top \leq \|G_j\|^2 \lambda_{\text{max}}(V) \leq B^2 \frac{v}{u^4} \leq C \frac{k^4}{u^4} \tau
$$

where $G_j$ denotes the $j$th row of $G$ and, as usual, $C > 0$ depends on $A$ only. The second inequality in the last display follows from property 3. in Definition 1 and by the definition of $B$ in (54), while the third inequality uses the first bound in Equation (78). The result follows from combining the previous bounds and the fact that $z_{\alpha/(2k)} = O(\sqrt{\log k})$. □

**Proof of Theorem 4.** We condition on $\mathcal{D}_{1,n}$ and the outcome of the sample splitting. The claimed results follows almost directly from Theorem 20, with few additional technicalities. The first difficulty is that the least squares estimator is not always well-defined under the bootstrap measure, which is the probability distribution of $n$ uniform draws with replacement from $\mathcal{D}_{2,n}$. In fact, any draw consisting of less than $d$ distinct elements of $\mathcal{D}_{2,n}$ will be such that the corresponding empirical covariance matrix will be rank deficient and therefore not invertible. On the other hand, because the distribution of $\mathcal{D}_{2,n}$ has a Lebesgue density by assumption, any set of $d$ or more points from $\mathcal{D}_{2,n}$ will be in general position and therefore will yield a unique set of least squares coefficients.

To deal with such complication we will simply apply Theorem 20 on the event that the bootstrap sample contains $d$ or more distinct elements of $\mathcal{D}_{2,n}$, whose complementary event, given the assumed scaling of $d$ and $n$, has probability is exponentially small in $n$, as shown next.

**Lemma 23.** For $d \leq n/2$, the probability that sampling with replacement $n$ out of $n$ distinct objects will result in a set with less than $d$ distinct elements is no larger than

$$
\exp \left\{ -\frac{n(1/2 - e^{-1})^2}{2} \right\}. \tag{80}
$$

**Remark.** The condition that $d \leq n/2$ can be replaced by the condition that $d \leq cn$, for any $c \in (0, 1 - e^{-1})$.

Thus, we will assume that the event that the bootstrap sample contains $d$ or more distinct elements of $\mathcal{D}_{2,n}$. This will result in an extra term that is of smaller order than any of the other terms and therefore can be discarded by choosing a larger value of the leading constant.

At this point, the proof of the theorem is nearly identical to the proof of Theorem 20 except for the way the term $A_3$ is handled. The assumptions that $n$ be large enough so that $v_n$ and $u_n$ are both positive implies, by Lemma 25 and Weyl’s theorem, that, for each $P \in \mathcal{P}^{\text{OLS}}_n$ and with probability at least $1 - \frac{2}{n}$ with respect to the distribution of $\mathcal{D}_{2,n}$, the bootstrap distribution belongs to the class $\mathcal{P}^*_n$ of probability distributions for the pair $(X, Y)$ that satisfy the properties of the probability distributions in the class $\mathcal{P}^{\text{OLS}}_n$ with two differences: (1) the quantities $U, u, v$ and $\bar{\tau}$ are replaced by $U_n, u_n, v_n$ and $\bar{\tau}_n$, respectively, and (2) the distributions in $\mathcal{P}^*_n$ need not have a Lebesgue density. Nonetheless, since the Lebesgue density assumption is only used to guarantee that empirical covariance matrix is invertible, a fact that is also true for the bootstrap distribution under the event that the bootstrap sample consists of $d$ or more distinct elements of $\mathcal{D}_{2,n}$, the bound on the term $A_3$ established in Theorem 20 holds for the larger class $\mathcal{P}^*_n$ as well.
Next, Lemma 22 can be used to bound the quantities \( \tilde{\sigma} \) and \( B \) for the class \( \mathcal{P}^*_n \). As for the bound on \( \mathcal{T} \), we proceed as in the proof of Theorem 2 and conclude that, for each non-empty subset \( S \) of \( \{1, \ldots, d\} \) and \( P \in \mathcal{P}^*_n \),

\[
\max_{j \in S} \int_0^1 \left\| H_j \left( (1-t)\psi_S(P) + t\hat{\psi}_S(P) \right) \right\|_{op} \, dt \leq \frac{C}{k} u_n^3
\]
on an event of probability at least \( 1 - \frac{1}{n} \), where \( C \) is the constant appearing in the second bound in (78). Thus, we may take \( \frac{C}{k} u_n^3 \) in lieu of \( \mathcal{T} \) and then apply Theorem 20 (noting that the high probability bound in the last display holds for each \( P \in \mathcal{P}^*_n \) separately).

**Proof of Theorem 6.** As remarked at the beginning of this appendix, throughout the proof all probabilistic statements will be made conditionally on the outcome of the splitting and on \( \mathcal{D}_{1,n} \). Thus, in particular, \( \hat{S} \) is to be regarded as a fixed subset of \( \{1, \ldots, d\} \) of size \( k \).

Let \( Z_n \sim N(0, \Sigma_{\hat{S}}) \), with \( \Sigma_{\hat{S}} \) given in 28. Notice that \( \Sigma_{\hat{S}} \) is almost surely positive definite, a consequence of adding extra noise in the definition of \( \gamma_{\hat{S}} \) and \( \hat{\gamma}_{\hat{S}} \). Then, using Theorem 2.1 in Chernozhukov et al. (2014), there exists a universal constant \( C > 0 \) such that

\[
\sup_{t=(t_j, j \in \hat{S}) \in \mathbb{R}_{+}^{|\hat{S}|}} \left| \mathbb{P}(\sqrt{n}|\hat{\gamma}_{\hat{S}}(j) - \gamma_{\hat{S}}(j)| \leq t_j, \forall j \in \hat{S}) - \mathbb{P}(|Z_n(j)| \leq t_j, \forall j \in \hat{S}) \right| \leq CE_{1,n}, \tag{81}
\]

where \( E_{1,n} \) is given in (33). By restricting the supremum in the above display to all \( t \in \mathbb{R}_{+}^{|\hat{S}|} \) with identical coordinates, we also obtain that

\[
\sup_{t > 0} \left| \mathbb{P}(\sqrt{n}||\hat{\gamma}_{\hat{S}} - \gamma_{\hat{S}}||_{\infty} \leq t) - \mathbb{P}(||Z_n||_{\infty} \leq t) \right| \leq CE_{1,n}. \tag{82}
\]

In order to show (31) and (32), we will use the same arguments used in the proofs of Theorem 18 and Theorem 19. We first define \( \mathcal{E}_n \) to be the event that

\[
\max_{i,j} \left| \hat{\Sigma}_{\hat{S}}(i,j) - \Sigma_{\hat{S}}(i,j) \right| \leq N_n, \tag{83}
\]

where \( N_n \) is as in (36). Each entry of \( \hat{\Sigma}_{\hat{S}} - \Sigma_{\hat{S}} \) is bounded in absolute value by \( (2(A + \tau) + \epsilon)^2 \), and therefore is a sub-Gaussian with parameter \( (2(A + \tau) + \epsilon)^4 \). Using a standard derivation for bounding the maximum of sub-Gaussian random variables we obtain that \( \mathbb{P}(\mathcal{E}_n^c) \leq \frac{1}{n} \). The bound (31) follows from the same arguments as in the proof Theorem 18: combine the Gaussian comparison Theorem 28 with (82) and notice that \( \epsilon / \sqrt{n} \) is a lower bound on the standard deviation of the individual coordinates of the \( \delta_i \)'s. In particular, the Gaussian comparison theorem yields the additional error term \( CE_{2,n} + \frac{1}{n} \) given in (34), for some universal positive constant \( C \). Similarly, (32) can be established along the lines of the proof of Theorem 19, starting from the bound (81). In this case we pick up an additional error term \( CE_{2,n} + \frac{1}{n} \) of different form, shown in (35), where \( C > 0 \) is a different universal constant.

Since all the bounds we have derived do not depend on \( \mathcal{D}_{1,n} \), the outcome of the splitting and \( w_n \), the same bounds therefore hold for the joint probabilities, and uniformly over the model selection and estimation procedures. The above arguments hold for each \( P \in \mathcal{P}^{\text{LOCO}}_n \). \( \square \)
Proof of Corollary 7. Following the proof of Corollary 3, for each $P \in \mathcal{P}_n^{\text{LOCO}}$ and on the event $\mathcal{E}_n$ given in (83) (which has probability at least $1 - \frac{1}{n}$), we have that

$$2 \max_{j \in \hat{S}} z_{\alpha/(2k)} \frac{\sqrt{\hat{\Sigma}(j,j)}}{n} \leq 2 \max_{j \in \hat{S}} z_{\alpha/(2k)} \frac{\Sigma_{\hat{S}}(j,j) + \hat{\Sigma}(j,j) - \Sigma(j,j)}{n} \leq z_{\alpha/(2k)} \sqrt{\frac{(2(A + \tau) + \epsilon)^2 + N_n}{n}}.$$ 

The claimed bound follows from the definition of $N_n$ as in (36). □

Proof of Theorem 8. All the probabilistic statements that follow are to be understood conditionally on the outcome of the sample splitting and on $\mathcal{D}_{1,n}$. Thus, $\mathcal{I}_{1,n}$, $\hat{S}$, $\hat{\beta}_{\hat{S}}$ and, for each $j \in \hat{S}$, $\hat{\beta}_{\hat{S}(j)}$ are to be regarded as fixed, and the only randomness is with respect to the joint marginal distribution of $\mathcal{D}_{2,n}$ and $(\xi_i, i \in \mathcal{I}_{2,n})$, and two auxiliary independent standard Gaussian vectors in $\mathbb{R}^{\hat{S}}$, $Z_1$ and $Z_2$, independent of everything else.

Let $\hat{\gamma}^*_{\hat{S}} \in \mathcal{R}^{\hat{S}}$ denotes the vector of LOCO parameters arising from the bootstrap distribution corresponding to the empirical measure associated to the $n$ triplets $\{(X_i, Y_i, \xi_i), i \in \mathcal{I}_{2,n}\}$.

Next,

$$\mathbb{P} \left( \sqrt{n} \| \hat{\gamma}_{\hat{S}} - \hat{\gamma}^*_{\hat{S}} \|_{\infty} \leq \hat{t}_{\alpha} \right) \geq \mathbb{P} \left( \sqrt{n} \| \hat{\gamma}_{\hat{S}} - \hat{\gamma}^*_{\hat{S}} \|_{\infty} \leq \hat{t}_{\alpha} \ | (X_i, Y_i, \xi_i), i \in \mathcal{I}_{2,n} \right) - (A_1 + A_2 + A_3),$$

where

$$A_1 = \sup_{t > 0} \left| \mathbb{P} \left( \sqrt{n} \| \hat{\gamma}_{\hat{S}} - \hat{\gamma}_{\hat{S}} \|_{\infty} \leq t \right) - \mathbb{P} (\| Z \|_{\infty} \leq t) \right|,$$

$$A_2 = \sup_{t > 0} \left| \mathbb{P} (\| Z \|_{\infty} \leq t) - \mathbb{P} (\| \hat{Z} \|_{\infty} \leq t) \right|,$$

and

$$A_3 = \sup_{t > 0} \left| \mathbb{P} \left( \sqrt{n} \| \hat{\gamma}_{\hat{S}} - \hat{\gamma}^*_{\hat{S}} \|_{\infty} \leq t \ | (X_i, Y_i, \xi_i), i \in \mathcal{I}_{2,n} \right) - \mathbb{P} (\| \hat{Z} \|_{\infty} \leq t) \right|,$$

with $Z = \Sigma_{\hat{S}}^{1/2} Z_1$ and $\hat{Z} = \hat{\Sigma}_{\hat{S}} Z_2$.

Then, $A_1 \leq C \mathbb{E}_{1,n}$ by (82) and $A_2 \leq C \mathbb{E}_{2,n} + \frac{1}{n}$, by applying the Gaussian comparison Theorem 28 on the event $\mathcal{E}_n$ that (83) holds, whereby $\mathbb{P}(\mathcal{E}_n) \leq \frac{1}{n}$ as argued in the proof of Theorem 6. Finally the bound on $A_3$ follows from applying Theorem 2.1 in Chernozhukov et al. (2014) to the bootstrap measure, conditionally on $(X_i, Y_i, \xi_i), i \in \mathcal{I}_{2,n}$, just like it was done in the proof of Theorem 6. In this case, we need to restrict to the even $\mathcal{E}_n$ to ensure that the minimal variance for the bootstrap measure is bounded away from zero. To that end, it will be enough to take $n$ large enough so that $\epsilon_n$ is positive and to replace $\epsilon$ with $\epsilon_n$. The price for this extra step is a factor of $\frac{1}{n}$, which upper bounds $\mathbb{P}(\mathcal{E}_n)$. Putting all the pieced together we arrive at the bound

$$A_3 \leq C \mathbb{E}_{1,n}^* + \frac{1}{n}.$$
Finally notice that $E_{1,n} \leq E_{1,n}^*$ since $\epsilon_n \leq \epsilon$.

The very same arguments apply to the other bootstrap confidence set $\tilde{C}^*_\alpha$, producing the very same bound. We omit the proof for brevity but refer the reader to the proof of Theorem 20 for details.

All the bounds obtained so far are conditionally on the outcome of the sample splitting and on $\mathcal{D}_{1,n}$ but are not functions of those random variables. Thus, the same bounds hold also unconditionally, for each $P \in \mathcal{P}_n^{\text{LOCO}}$.

$\square$

Let $F_{n,j}$ denote the empirical cumulative distribution function of $\{\delta_i(j), i \in \mathcal{I}_{2,n}\}$ and $F_j$ the true cumulative distribution function of $\delta_i(j)$. Thus, setting $\beta_l = l/n$ and $\beta_u = u/n$, we see that $\delta_l(j) = F_{n,j}^{-1}(\beta_l)$ and $\delta_u(j) = F_{n,j}^{-1}(\beta_u)$ and, furthermore, that $F_{n,j}(F_{n,j}^{-1}(\beta_l)) = \beta_l$ and $F_{n,j}(F_{n,j}^{-1}(\beta_u)) = \beta_u$. In particular notice that $\beta_l$ is smaller than $\frac{1}{2} - \sqrt{\frac{1}{2n} \log \left(\frac{2k}{\alpha}\right)}$ by at most $1/n$ and, similarly, $\beta_u$ is larger than $\frac{1}{2} + \sqrt{\frac{1}{2n} \log \left(\frac{2k}{\alpha}\right)}$ by at most $1/n$.

By assumption, the median $\mu_j = F_j^{-1}(1/2)$ of $\delta_i(j)$ is unique and the derivative of $F_j$ is larger than $M$ at all points within a distance of $\eta$ from $\mu_j$. Thus, by the mean value theorem, we must have that, for all $x \in \mathbb{R}$ such that $|x - \mu_j| < \eta$,

$$ M|x - \mu_j| \leq |F_j(x) - F_j(\mu_j)|. $$

As a result, if

$$ |F_j(x) - F_j(\mu_j)| \leq M\eta, \quad (84) $$

it is the case that $|x - \mu_j| \leq \eta$, and therefore, that $|x - \mu_j| \leq \frac{F_j(x) - F_j(\mu_j)}{M}$. By the DKW inequality and the union bound, with probability at least $1 - 1/n$,

$$ \max_{j \in \tilde{S}} \|F_{n,j} - F_j\|_\infty \leq \sqrt{\frac{\log 2kn}{2n}}. \quad (85) $$

Thus, for any $j \in \tilde{S}$,

$$ |F_{n,j}(\delta_u(j)) - F_j(\delta_u(j))| \leq \sqrt{\frac{\log 2kn}{2n}}. $$

Since

$$ F_{n,j}(\delta_u(j)) = \beta_u \leq 1/2 + \frac{1}{n} \sqrt{\frac{1}{n} \log \left(\frac{2k}{\alpha}\right)} = F_j(\mu_j) + \frac{1}{n} \sqrt{\frac{1}{n} \log \left(\frac{2k}{\alpha}\right)}, $$

using (84), we conclude that, on the event (85) and provided that

$$ \frac{1}{n} \sqrt{\frac{1}{n} \log \left(\frac{2k}{\alpha}\right)} + \sqrt{\frac{\log 2kn}{2n}} \leq \eta M, $$

$$ |\mu_j - \delta_u(j)| \leq \frac{1}{M} \left( \frac{1}{n} + \sqrt{\frac{1}{n} \log \left(\frac{2k}{\alpha}\right)} + \sqrt{\frac{\log 2kn}{2n}} \right). $$

Similarly, under the same conditions,

$$ |\mu_j - \delta_l(j)| \leq \frac{1}{M} \left( \frac{1}{n} + \sqrt{\frac{1}{n} \log \left(\frac{2k}{\alpha}\right)} + \sqrt{\frac{\log 2kn}{2n}} \right). $$
The claim now follows by combining the last two displays. Notice that the result holds uniformly over all \( j \in \hat{S} \) and all distributions satisfying the conditions of the theorem. \( \square \)

10 Appendix 3: Proof of the results in Section 3

Proof of Lemma 11. The upper bounds are obvious. The lower bound (44) is from Section 4 in Sackrowitz and Samuel-Cahn (1986). We now show (46). Let \( \hat{\beta} = g(Y) \) be any estimator where \( Y = (Y_1, \ldots, Y_n) \). Given any \( Y \) and any \( w(Y) \), \( \hat{\beta} \) provides an estimate of \( \beta(J) \) where \( J = w(Y) \). Let \( w_j \) be such that \( w_j(X) = j \). Then define \( \hat{\beta} = (g(Y, w_1(Y)), \ldots, g(Y, w_D(Y))) \). Let \( w_0(Y) = \arg\max_j |\beta(j) - \hat{\beta}(j)| \). Then \( \mathbb{E}[|\hat{\beta}(J) - \beta(J)|] = \mathbb{E}[|\|\hat{\beta} - \beta\|_\infty] \). Let \( P_0 \) be multivariate Normal with mean \((0, \ldots, 0)\) and identity covariance. For \( j = 1, \ldots, D \) let \( P_j \) be multivariate Normal with mean \( \mu_j = (0, \ldots, 0, a, 0, 0) \) and identity covariance where \( a = \sqrt{\log D/(16n)} \). Then

\[
\inf_{\hat{\beta}} \sup_{w \in W_n} \sup_{P \in P_n} \mathbb{E}[|\hat{\beta}(J) - \beta(J)|] \geq \inf_{\hat{\beta}} \sup_{P \in M} \mathbb{E}[|\|\hat{\beta} - \beta\|_\infty]
\]

where \( J = w_0(Y) \) and \( M = \{P_0, P_1, \ldots, P_D\} \). It is easy to see that

\[
\text{KL}(P_0, P_j) \leq \frac{\log D}{16n}
\]

where KL denotes the Kullback-Leibler distance. Also, \( ||\mu_j - \mu_k||_\infty \geq a/2 \) for each pair. By Theorem 2.5 of Tsybakov (2009),

\[
\inf_{\hat{\beta}} \sup_{P \in M} \mathbb{E}[||\hat{\mu} - \mu||_\infty] \geq \frac{a}{2}
\]

which completes the proof. \( \square \)

Proof of Lemma 14. We use a contiguity argument like that in Leeb and Pötscher (2008). Let \( Z_1, \ldots, Z_D \sim N(0,1) \). Note that \( \hat{\beta}(j) \overset{d}{=} \beta(j) + Z_j/\sqrt{n} \). Then

\[
\psi_n(\beta) = \mathbb{P}(\sqrt{n}(\hat{\beta}(S) - \beta(S)) \leq t) = \sum_j \mathbb{P}(\sqrt{n}(\hat{\beta}(j) - \beta(j)) \leq t, \hat{\beta}(j) > \max_{s \neq j} \hat{\beta}_s) = \sum_j \mathbb{P}(\max_{s \neq j} Z_s + \sqrt{n}(\beta(s) - \beta(j)) < Z_j < t) = \sum_j \Phi(A_j)
\]

where \( \Phi \) is the \( d \)-dimensional standard Gaussian measure and

\[
A_j = \left\{ \max_{s \neq j} Z_s + \sqrt{n}(\beta(s) - \beta(j)) < Z_j < t \right\}.
\]

Consider the case where \( \beta = (0, \ldots, 0) \). Then

\[
\psi_n(0) = D \Phi(\max_{s \neq 1} Z_s < Z_1 < t) \equiv b(0).
\]
Next consider \( \beta_n = (a/\sqrt{n}, 0, 0, \ldots, 0) \) where \( a > 0 \) is any fixed constant. Then

\[
\psi(\beta_n) = \Phi((\max_{s \neq 1} Z_s) - a < Z_1 < t)
\]

\[
+ \sum_{j=2}^{D} \Phi(\max\{Z_1 + a, Z_2, \ldots, Z_{j-1}, Z_{j+1}, \ldots, Z_D\} < Z_j < t)
\]

\[
\equiv b(a).
\]

Suppose that \( \hat{\psi}_n \) is a consistent estimator of \( \psi_n \). Then, under \( P_0, \hat{\psi}_n \xrightarrow{P} b(0) \). Let \( P_n = N(\beta_n, I) \) and \( P_0 = N(0, I) \). It is easy to see that \( P_0^n(A_n) \to 0 \) implies that \( P_n^n(A_n) \to 0 \) so that \( P_n \) and \( P_0 \) are contiguous. So, by Le Cam’s first lemma (see, e.g. Bickel et al., 1998), under \( P_n \), we also have that \( \hat{\psi}_n \xrightarrow{P} b(0) \). But \( b(0) \neq b(a) \), which contradicts the assumed consistency of \( \hat{\psi}_n \). □

**Proof of Lemma 15.** Let \( P_0 = N(\mu_0, \frac{1}{n} I_D) \), where \( \mu_0 = 0 \), and for \( j = 1, \ldots, D \) let \( P_j = N(\mu_j, \frac{1}{n} I_D) \), where \( \mu_j \) is the \( D \)-dimensional vector with 0 entries except along the \( j \)th coordinate, which takes the value \( \sqrt{c \log \frac{D}{n}} \), where \( 0 < c < 1 \). Consider the mixture \( \bar{P} = \frac{1}{P} \sum_{j=1}^{D} P_j \). Then, letting \( \theta_j \) and \( \theta_0 \) be the largest coordinates of \( \mu_j \) and \( \mu_0 \) respectively, we have that \( \|\theta_j - \theta_0\|^2 = \frac{c \log D}{n} \) for all \( j \). Next, some algebra yields that the \( \chi^2 \) distance between \( P_0 \) and the mixture \( \overline{P} = \frac{1}{P} \sum_{j=1}^{D} P_j \) is \( \frac{1}{P} \sqrt{c \log D} - \frac{1}{P} \), which vanishes as \( D \) tends to \( \infty \). Since this is also an upper bound on the squared total variation distance between \( P_0 \) and \( \overline{P} \), the result follows from an application of Le Cam Lemma (see, e.g. Tsybakov, 2009). □

11 Appendix 4: Proof of the results in Section 6

**Proof of Theorem 16.** For ease of readability, we will write \( G_j \) and \( G \) instead of \( G_j(\psi) \) and \( G(\psi) \), respectively. Throughout the proof, \( C \) will indicate a positive number whose value may change from line to line and which depends on \( A \) only, but on none of the remaining variables.

For each \( j \in \{1, \ldots, s\} \), we use a second order Taylor expansion of \( \hat{\theta}_j \) to obtain that

\[
\hat{\theta}_j = \theta_j + G_j(\hat{\psi} - \psi) + \frac{1}{2n} \delta^\top \Lambda_j \delta, \quad \forall j \in \{1, \ldots, s\}
\]

where \( \delta = \sqrt{n}(\hat{\psi} - \psi) \) and \( \Lambda_j = \int_0^1 H_j((1-t)\psi + t\hat{\psi})dt \in \mathbb{R}^{b \times b} \). Hence,

\[
\sqrt{n}(\hat{\theta} - \theta) = \sqrt{n}(\hat{\psi} - \psi) + R
\]

where \( \nu = G\psi, \hat{\nu} = G\hat{\psi} \) and \( R \) is a random vector in \( \mathbb{R}^s \) whose \( j \)th coordinate is

\[
R_j = \frac{1}{2\sqrt{n}} \delta^\top \left[ \int_0^1 H_j((1-t)\psi + t\hat{\psi})dt \right] \delta.
\]

By Lemma 24 below, there exists a constant \( C > 0 \), depending on \( A \) only, such that

\[
\sup_{P \in \mathcal{P}_n} \sup_{t} \left| \mathbb{P}(\sqrt{n}\|\hat{\nu} - \nu\|_{\infty} \leq t) - \mathbb{P}(\|Z_n\|_{\infty} \leq t) \right| \leq C \frac{1}{\sqrt{v}} \left( \frac{\pi^2 b(\log 2bn)^7}{n} \right)^{1/6},
\]

\[
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\]
where $Z_n \sim N_s(0, \Gamma)$.

Now we bound the effect of remainder $R$ in (86). First, by assumption (see Equation 54), we have that, almost everywhere,

$$\sup_{u \in [0,1]} \| H_j((1-u)\psi + u\hat{\psi}) \|_{op} \leq \overline{H},$$

from which it is follows that

$$\|R\|_{\infty} \leq \frac{\overline{H}||\delta||^2}{2\sqrt{n}},$$

with the inequality holding uniformly in $P_n$. Next, consider the event

$$E_n = \{ \left| |\hat{\psi} - \psi| \right| > \sqrt{2\epsilon_n \sqrt{n\overline{H}}} \}$$

for a sufficiently large, positive constant $C$ to be specified later. Thus, since $\delta = \sqrt{n}(\hat{\psi} - \psi)$, we have that

$$P(E^c_n) = P\left( \frac{\overline{H}||\delta||^2}{2\sqrt{n}} > \epsilon_n \right)$$

where the inequality follows from (86) and the fact that $\|R\|_{\infty} \leq \epsilon_n$ on the event $E_n$ and the second identity from the Berry-Esseen bound (87). By the Gaussian anti-concentration inequality of Theorem 26,

$$P(|Z_n|_{\infty} \leq t + \epsilon_n) \leq P(|Z_n|_{\infty} \leq t) + \frac{\epsilon_n}{\sqrt{2\log b + 2}}.$$
Using the previous inequality on the first term of (91), we obtain that
\[
\mathbb{P}(\sqrt{n}|\hat{\theta} - \theta|_\infty \leq t) \leq \mathbb{P}(\|Z_n\|_\infty \leq t) + C \left[ \frac{\epsilon_n}{\sigma} (\sqrt{2 \log b} + 2) + \frac{1}{\sqrt{v}} \left( \frac{v^2 b \log (2bn)^7}{n} \right)^{1/6} \right] + \mathbb{P}(\mathcal{E}_n^c),
\]
where in the second inequality we have used the fact that \(\mathbb{P}(\mathcal{E}_n^c) \leq \frac{1}{n}\) by (90) and have absorbed this lower order term into higher order terms by increasing the value of \(C\). By a symmetric argument, we have
\[
\mathbb{P}(\sqrt{n}|\hat{\theta} - \theta|_\infty \leq t) \geq \mathbb{P}(\|Z_n\|_\infty \leq t) - C \left[ \frac{\epsilon_n}{\sigma} (\sqrt{2 \log b} + 2) + \frac{1}{\sqrt{v}} \left( \frac{v^2 b \log (2bn)^7}{n} \right)^{1/6} \right],
\]
The result now follows by bounding \(\epsilon_n\) as in (89). □

The following lemma shows that the linear term \(\sqrt{n} (\hat{\nu} - \nu)\) in (86) has a Gaussian-like behavior and is key ingredient of our results. It is an application of the Berry-Esseen Theorem 27, due to Chernozhukov et al. (2014). The proof is in Section 12.

**Lemma 24.** There exists a constant \(C > 0\), depending on \(A\) only, such that
\[
\sup_{P \in \mathcal{P}} \sup_{t} \left| \mathbb{P}(\sqrt{n}|\hat{\nu} - \nu|_\infty \leq t) - \mathbb{P}(\|Z_n\|_\infty \leq t) \right| \leq C \left[ \frac{1}{\sqrt{v}} \left( \frac{v^2 b \log (2bn)^7}{n} \right)^{1/6} \right],
\]
where \(Z_n \sim N_s(0, \Gamma)\).

**Proof of Lemma 17.** Throughout the proof, we set \(G = G(\psi)\), where \(\psi = \psi(P)\) for some \(P \in \mathcal{P}_n\), and \(\hat{G} = G(\hat{\psi})\) where \(\hat{\psi} = \hat{\psi}(P)\) is the sample average from an i.i.d. sample from \(P\). Recall that the matrices \(\Gamma\) and \(\hat{\Gamma}\) are given in Equations (56) and (61), respectively. For convenience we will suppress the dependence of \(\hat{\Gamma}\) and \(\hat{G}\), and of \(\Gamma\) and \(G\) on \(\psi\) and \(\hat{\psi}\), respectively.

Express \(\hat{\Gamma} - \Gamma\) as
\[
(\hat{G} - G)VG^\top + GV(\hat{G} - G)^\top + (\hat{G} - G)V(\hat{G} - G)^\top + (\hat{G} - G)(\hat{V} - V)(\hat{G} - G)^\top + G(\hat{V} - V)G^\top + (\hat{G} - G)(\hat{V} - V)^\top (\hat{G} - G)^\top.
\]
The first, second and sixth terms are dominant, so it will be enough to compute high-probability bounds for \((\hat{G} - G)VG^\top\) and \(G(\hat{V} - V)G^\top\).

We first bound \((\hat{G} - G)VG^\top\). For any \(j\) and \(l\) in \(\{1, \ldots, s\}\) and using the Cauchy-Schwartz inequality, we have that
\[
\left| (\hat{G}_j - G_j) VG_{l}^\top \right| \leq \lambda_{\max}(V) \| \hat{G}_j - G_j \| B \leq \pi B \| \hat{G}_j - G_j \|,
\]
by the definition of \(B\) (see Equation 54), where we recall that \(G_j\) denotes the \(j\)th row of \(G\).
It remains to bound the stochastic term \( \max_j \| \hat{G}_j - G_j \| \). Towards that end, we will show that, for some constant \( C \) dependent on \( A \) only,

\[
P \left( \max_j \| \hat{G}_j - G_j \| \leq C \bar{H} \sqrt{b \log n / n} \right) \geq 1 - 1/n. \tag{94}
\]

Indeed, by a Taylor expansion,

\[
\hat{G}_j - G_j = \left( \hat{\psi} - \psi \right)^\top \int_0^1 H_j((1 - t)\psi + t\hat{\psi}) dt \quad \text{for all} \quad j \in \{1, \ldots, s\},
\]

so that

\[
\max_j \| \hat{G}_j - G_j \| \leq \| \psi - \hat{\psi} \| \max_j \left\| \int_0^1 H_j((1 - t)\psi + t\hat{\psi}) dt \right\|_{\text{op}}.
\]

Since the coordinates of \( \hat{\psi} \) are bounded in absolute value by \( A \), the bound (103) implies that, for some positive constant \( C \) dependent on \( A \) only,

\[
P \left( \| \hat{\psi} - \psi \| \leq C \sqrt{b \log n / n} \right) \geq 1 - 1/n,
\]

for all \( P \in \mathcal{P}_n^{\text{OLS}} \). We restrict to this event. By convexity of the operator norm \( \| \cdot \|_{\text{op}} \) and our assumption, we have that

\[
\max_j \left\| \int_0^1 H_j((1 - t)\psi + t\hat{\psi}) dt \right\|_{\text{op}} \leq \bar{H}, \tag{95}
\]

yielding the bound in (94). Combined with (93), we conclude that on an event of probability at least \( 1 - 1/n \), \( \max_{j,l} | \hat{\Gamma}(j,l) - \Gamma(j,l) | \leq \tilde{\ell}_n \). This bound holds uniformly over \( P \in \mathcal{P}_n \).

As for the other term \( G(\hat{V} - V)G^\top \), we have that, by (104) in Lemma 25,

\[
\max_{j,l} \left| G_j(\hat{V} - V)G_l^\top \right| \leq B^2\| \hat{V} - V \|_{\text{op}} \leq CB^2 \sqrt{b \log b + \log n},
\]

with probability at least \( 1 - \frac{1}{n} \), where \( C \) depends only on \( A \) and we have used the fact that \( \max_j \| G_j(\psi(P)) \|^2 \leq B^2 \) uniformly over \( P \in \mathcal{P}_n \).

Thus, by a union bound, the claim holds on an event of probability at least \( 1 - \frac{2}{n} \). \( \square \)

**Proof of Theorem 18.** Let \( Z_n \sim N(0, \Gamma) \) and recall that \( \hat{Z}_n \sim N(0, \hat{\Gamma}) \). Using the triangle inequality, we have that

\[
P(\theta \in \hat{C}_n) = P(\sqrt{n}||\hat{\theta} - \theta||_\infty \leq \hat{\ell}_n) \geq P(||\hat{Z}_n||_\infty \leq \hat{\ell}_n) - A_1 - A_2,
\]

where

\[
A_1 = \sup_{t > 0} | P(\sqrt{n}||\hat{\theta} - \theta||_\infty \leq t) - P(||Z_n||_\infty \leq t) |
\]

and

\[
A_2 = \sup_{t > 0} | P(||Z_n||_\infty \leq t) - P(||\hat{Z}_n||_\infty \leq t) |.
\]

Now

\[
P(||\hat{Z}_n||_\infty \leq \hat{\ell}_n) = E[P(||\hat{Z}_n||_\infty \leq \hat{\ell}_n|\hat{\Gamma})] = 1 - \alpha,
\]

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by the definition of $\hat{t}_n$. Theorem 16 implies that $A_1 \leq C(\Delta_{1,n} + \Delta_{2,n})$, where $C$ depends on $A$ only. To bound $A_2$, consider the event $\mathcal{E}_n = \{\max_{j,k} |\hat{t}_j - \hat{t}_k| \leq Cn\}$, where the constant $C$ is the same as in Lemma 17. Then, by the same Lemma, $P(\mathcal{E}_n) \geq 1 - 1/n$, uniformly over all $P$ in $\mathcal{P}_n$. Next, we have that

$$A_2 \leq \mathbb{E} \left[ \sup_{t > 0} \left( \mathbb{P}(||Z_n||_\infty \leq t) - \mathbb{P}(||\hat{Z}_n||_\infty \leq t) \right) \right] + \mathbb{P}(\mathcal{E}_n^c),$$

where $\mathbb{E}[;\mathcal{E}_n]$ denotes expectation restricted to the event $\mathcal{E}_n$. By the Gaussian comparison Theorem 28 the term inside the expected value is bounded by $\Delta_n$. □

**Proof of Theorem 19.** For $j = 1, \ldots, s$, let $\gamma_j = \sqrt{\Gamma_{j,j}}$, $\hat{\gamma}_j = \sqrt{\Gamma_{j,j}}$, and $\hat{t}_j = z_{\alpha/(2s)}\hat{\gamma}_j$. We use the same arguments and notation as in the proofs of Theorem 16 and Lemma 24. Thus, let $\mathcal{E}_n$ be the event that $\frac{||\delta||^2}{2\sqrt{n}} < \epsilon_n$, where $\frac{||\delta||^2}{2\sqrt{n}}$ is an upper bound on $||R||_\infty$, with $R$ the reminder in the Taylor series expansion (86) and $\epsilon_n$ as in (89). Then, $\mathbb{P}(\mathcal{E}_n^c) \leq n^{-1}$ (see equation 90).

Next, for each $t \in \mathbb{R}^{2s}$ and any Jacobian matrix $G = G(\psi(P))$, with $P \in \mathcal{P}_n$, let

$$P(G, t) = \left\{ x \in \mathbb{R}^b : v^T_l x \leq t_l, \forall v_l \in \mathcal{V}(G) \right\},$$

where $\mathcal{V}(G)$ is defined in the proof of Lemma 24. Then, for any positive numbers $(t_1', \ldots, t_s')$

$$|\sqrt{n}(\hat{\nu}_j - \nu_j)| \leq t_j', \quad j = 1, \ldots, s \quad \text{if and only if} \quad \sqrt{n}(\hat{\psi} - \psi) \in P(G, t),$$

where the coordinates of $t \in \mathbb{R}^{2s}$ are as follows: for $j = 1, \ldots, s$, $t_{2l-1} = t_{2l} = \frac{t_j'}{\|v_j\|}$. Consider now the class of subsets of $\mathbb{R}^b$ of the form specified in (96), where $t$ ranges over the positive vectors in $\mathbb{R}^{2s}$ and $G$ ranges in $\{G(\psi(P)), P \in \mathcal{P}_n\}$. This is a class comprised by polytopes with at most $2s$ faces in $\mathbb{R}^b$. Thus, using the same arguments as in the proof of Lemma 24, we obtain that

$$\sup_{t = (t_1', \ldots, t_s') \in \mathbb{R}^s_+} \left[ \mathbb{P}\left( \sqrt{n}(\hat{\nu}_j - \nu_j) \leq t_j, \forall j \right) - \mathbb{P}\left( \{Z_{n,j} \leq t_j, \forall j \} \right) \right] \leq C \frac{1}{\sqrt{v}} \left( \frac{v^2 b (\log 2b)^7}{n} \right)^{1/6},$$

for some $C > 0$ depending only on $A$, where $Z_n \sim N(0, \Gamma)$. Using the above display, and following the same arguments as in the proof of Theorem 16, we have that

$$\mathbb{P}(\sqrt{n}(\hat{\theta}_j - \theta_j) \leq \hat{t}_j, \forall j) = \mathbb{P}(\sqrt{n}(\hat{\theta}_j - \theta_j) \leq \hat{t}_j, \forall j; \mathcal{E}_n) + \mathbb{P}(\sqrt{n}(\hat{\theta}_j - \theta_j) \leq \hat{t}_j, \forall j; \mathcal{E}_n^c)$$

$$\leq \mathbb{P}(\sqrt{n}(\hat{\nu}_j - \nu_j) \leq \hat{t}_j + \epsilon_n, \forall j) + \mathbb{P}(\mathcal{E}_n^c)$$

$$\leq \mathbb{P}(\{Z_{n,j} \leq \hat{t}_j + \epsilon_n, \forall j\}) + \mathbb{P}(\mathcal{E}_n^c)$$

$$\leq \mathbb{P}(\{Z_{n,j} \leq \hat{t}_j, \forall j\}) + C \left[ \frac{\epsilon_n}{\alpha} (\sqrt{2\log b} + 3) + \frac{1}{\sqrt{v}} \left( \frac{v^2 b (\log 2b)^7}{n} \right)^{1/6} \right],$$

where in the second-to-last inequality we have used the fact that $\mathbb{P}(\mathcal{E}_n^c) \leq \frac{1}{n}$ and in the last inequality we have applied the Gaussian anti-concentration inequality in Theorem 26 (and have absorbed the term $\frac{1}{n}$ into higher order terms by increasing the value of $C$). A similar argument gives

$$\mathbb{P}(\sqrt{n}(\hat{\theta}_j - \theta_j) \leq \hat{t}_j, \forall j) \geq \mathbb{P}(\{Z_{n,j} \leq \hat{t}_j, \forall j\}) - C \left[ \frac{\epsilon_n}{\alpha} (\sqrt{2\log b} + 3) + \frac{1}{\sqrt{v}} \left( \frac{v^2 b (\log 2b)^7}{n} \right)^{1/6} \right].$$

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To complete the proof, we will show that
\[
\mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) \geq (1 - \alpha) - \frac{1}{n} - \min \left\{ C \Delta_{3,n}, \frac{8n z_{\alpha/(2s)}}{(\min_j \gamma_j)^2} \left( \sqrt{2 + \log(2)} + 2 \right) \right\}.
\]
(98)

Let \( \tilde{Z}_n \sim N(0, \hat{\Gamma}) \). By the Gaussian comparison Theorem 28,
\[
\mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) \geq \mathbb{P}(|\tilde{Z}_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) - I \geq 1 - \alpha - I
\]
where
\[
I = \mathbb{E} \left[ \sup_{t = (t_1, \ldots, t_s) \in \mathbb{R}^s_+} \left| \mathbb{P}(|Z_{j,n}| \leq t_j, \forall j) - \mathbb{P}(|\tilde{Z}_{j,n}| \leq t_j, \forall j)|F_n \right| \right] + \mathbb{P}(F_n^c) \leq C \Delta_{3,n} + \frac{1}{n}.
\]

In the above expression the constant \( C \) is the same as in Lemma 17 and \( F_n \) is the event that \( \{ \max_{j,k} |\hat{\Gamma} - \Gamma| \leq C \hat{n} \} \), which is of probability at least \( 1 - \frac{1}{\hat{n}} \), again by Lemma 17. This gives the first bound in (98).

To prove the second bound in (98) we let \( \Xi_n = C \frac{8n}{\min_j \gamma_j} \), where \( C \) is the constant in Lemma 17, and then notice that, on the event \( F_n \),
\[
|\gamma_j - \hat{\gamma}_j| = \frac{|\gamma_j^2 - \hat{\gamma}_j^2|}{|\gamma_j + \hat{\gamma}_j|} \leq \frac{|\hat{\gamma}_j^2 - \gamma_j^2|}{\gamma_j} \leq \frac{\max_j |\hat{\gamma}_j^2 - \gamma_j^2|}{\min_j \gamma_j} \leq \Xi_n.
\]
Thus,
\[
\mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) = \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \hat{\gamma}_j, \forall j) - \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) \geq \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \hat{\gamma}_j, \forall j; F_n) - \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) + \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j)
\]
\[
\geq \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \hat{\gamma}_j, \forall j; F_n) - \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) + (1 - \alpha),
\]
where in the last step we have used the union bound. Next,
\[
\mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \hat{\gamma}_j, \forall j; F_n) = \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} (\gamma_j - \Xi_n), \forall j; F_n) \geq \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} (\gamma_j - \Xi_n), \forall j) - \mathbb{P}(F_n^c).\]
Thus,
\[
\mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \hat{\gamma}_j, \forall j) \geq (1 - \alpha) - \mathbb{P}(F_n^c) + \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} (\gamma_j - \Xi_n), \forall j) - \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j)
\]
\[
\geq (1 - \alpha) - \frac{1}{n} - \frac{\Xi_n z_{\alpha/(2s)}}{\min_j \gamma_j} \left( \sqrt{2 + \log(2)} + 2 \right),
\]
since, by the Gaussian anti-concentration inequality of Theorem 26,
\[
\mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} (\gamma_j - \Xi_n), \forall j) - \mathbb{P}(|Z_{n,j}| \leq z_{\alpha/(2s)} \gamma_j, \forall j) \geq - \frac{\Xi_n z_{\alpha/(2s)}}{\min_j \gamma_j} \left( \sqrt{2 + \log(2)} + 2 \right).
\]
The result follows by combining all the above bounds and the fact that \( \sigma^2 = \min_{P \in \mathcal{P}_n} \min_j \Gamma(j, j) \).
As usual, we have absorbed any lower order term (namely \( \frac{1}{n} \)) into higher order ones. \( \square \)
Proof of Theorem 20. Let $Z_n \sim N(0, \Gamma)$ where $\Gamma = GVG^T$ and $\hat{Z}_n \sim N(0, \hat{\Gamma})$ where we recall that $\hat{\Gamma} = \hat{G}V\hat{G}^T$, $\hat{G} = G(\hat{\psi})$ and $\hat{V} = n^{-1}\sum_{i=1}^n(W_i - \hat{\psi})(W_i - \hat{\psi})^T$. Take $\mathcal{E}_n$ to be the event that

$$\left\{ \max_{j,k} | \hat{\Gamma} - \Gamma | \leq C\mathcal{N}_n \right\} \cap \{ \| V - \hat{V} \|_{op} \leq C\mathcal{T}_n \},$$

where $C$ is the larger of the two constants in (63) and in (104). Then, by Lemma 17 and Lemma 25, $\mathbb{P}(\mathcal{E}_n) \geq 1 - 2/n$, uniformly over all the distributions in $\mathcal{P}_n$. By the triangle inequality,

$$\mathbb{P}(\theta \in \hat{C}_n^*) = \mathbb{P}(\sqrt{n}||\hat{\theta} - \theta||_\infty \leq \hat{t}_n^*) \geq \mathbb{P}(\sqrt{n}||\hat{\theta}^* - \Theta||_\infty \leq \hat{t}_n^*(W_1, \ldots, W_n)) - (A_1 + A_2 + A_3),$$

(99)

where

$$A_1 = \sup_{t > 0} \left| \mathbb{P}\left(\sqrt{n}||\hat{\theta} - \theta||_\infty \leq t \right) - \mathbb{P}(\| Z_n \|_\infty \leq t) \right|,$$

$$A_2 = \sup_{t > 0} \left| \mathbb{P}(\| Z_n \|_\infty \leq t) - \mathbb{P}(\| \hat{Z}_n \|_\infty \leq t) \right|,$$

and

$$A_3 = \sup_{t > 0} \left| \mathbb{P}(\| \hat{Z}_n \|_\infty \leq t) - \mathbb{P}\left(\sqrt{n}||\hat{\theta}^* - \hat{\theta}||_\infty \leq t \right) \right|.$$

Since, by definition, $\mathbb{P}(\sqrt{n}||\hat{\theta}^* - \hat{\theta}||_\infty \leq \hat{t}_n^*(W_1, \ldots, W_n)) \geq 1 - \alpha$, it follows from (99) that, in order to establish (71) we will need to upper bound each of the terms $A_1$, $A_2$ and $A_3$ accordingly. The term $A_1$ has already been bounded by $C(\Delta_{1,n} + \Delta_{2,n})$ in the earlier Theorem 16. For $A_2$ we use the Gaussian comparison Theorem 28 as in the proof of Theorem 18 restricted to the event $\mathcal{E}_n$ to conclude that $A_2 \leq C\Delta_{n,3} + \frac{2}{n}$. Finally, to bound $A_3$, one can apply the same arguments as in Theorem 16, but restricted to the event $\mathcal{E}_n$, to the larger class of probability distributions $\mathcal{P}_n^*$ differing from $\mathcal{P}_n$ only in the fact that $v$ is replaced by the smaller quantity $v_n > 0$ and $\Psi$ by the larger quantity $\Psi_n = \Psi + C\mathcal{T}_n$. In particular, the bootstrap distribution belongs to $\mathcal{P}_n^*$. In detail, one can replace $\psi$ and with $\hat{\psi}$, and $\hat{\psi}$ with $\hat{\psi}^*$ and, similarly, $\Gamma$ with $\hat{\Gamma}$ and $\hat{\Gamma}$ with $\hat{\Gamma}^* = G(\hat{\psi}^*)\hat{V}^*G(\hat{\psi}^*)^T$, where $\hat{V}^*$ is the empirical covariance matrix based on a sample of size $n$ from the bootstrap distribution. The assumption that $n$ is large enough so that $v_n$ and $\sigma_n^2$ are positive ensures that, on the event $\mathcal{E}_n$ of probability at least $1 - 2/n$, $\min_j \sqrt{\hat{\Gamma}(j,j)} > \sqrt{\sigma_n^2 - C\mathcal{N}_n} > 0$ and, by Weyl’s inequality, the minimal eigenvalue of $\hat{V}$ is no smaller than $v - C\mathcal{T}_n > 0$. In particular, the error terms $\Delta_{n,1}^*$ and $\Delta_{n,2}^*$ are well-defined (i.e. positive). Thus we have that

$$A_3 \leq C(\Delta_{n,1}^* + \Delta_{n,2}^*) + \frac{2}{n},$$

(100)

where the lower order term $\frac{1}{n}$ is reported to account for the restriction to the event $\mathcal{E}_n$. The result now follows by combining all the bounds, after noting that $\Delta_{1,n} \leq \Delta_{1,n}^*$ and $\Delta_{2,n} \leq \Delta_{2,n}^*$. To show that the same bound holds for the coverage of $C_n^*$ we proceed in a similar manner. Using the triangle inequality, and uniformly over all the distributions in $\mathcal{P}_n$,

$$\mathbb{P}(\theta \in \hat{C}_n^*) = \mathbb{P}(\sqrt{n}|\hat{\theta}_j - \theta_j| \leq \hat{t}_{j,\alpha}^*, \forall j) \geq \mathbb{P}\left(\sqrt{n}|\hat{\theta}_j^* - \hat{\theta}_j| \leq \hat{t}_{j,\alpha}^*, \forall j \left| (W_1, \ldots, W_n) \right\} - (A_1 + A_2 + A_3) \right.$$

$$\geq (1 - \alpha) - (A_1 + A_2 + A_3),$$

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where

\[ A_1 = \sup_{t = (t_1, \ldots, t_s) \in \mathbb{R}_+^s} \left| \mathbb{P}\left( \sqrt{n} |\hat{\theta}_j - \theta_j| \leq t_j, \forall j \right) - \mathbb{P}(|Z_{n,j}| \leq t_j, \forall j) \right|, \]

\[ A_2 = \sup_{t = (t_1, \ldots, t_s) \in \mathbb{R}_+^s} \left| \mathbb{P}(|Z_{n,j}| \leq t_j, \forall j) - \mathbb{P}(\hat{Z}_{n,j} \leq t_j, \forall j) \right|, \]

and

\[ A_3 = \sup_{t = (t_1, \ldots, t_s) \in \mathbb{R}_+^s} \left| \mathbb{P}(\hat{Z}_{n,j} \leq t_j, \forall j) - \mathbb{P}\left( \sqrt{n} |\hat{\theta}_j^* - \hat{\theta}_j| \leq t_j, \forall j \right| (W_1, \ldots, W_n) \right|. \]

The term \( A_1 \) is bounded by \( C(\Delta_{1,n} + \Delta_{2,n}) \), as shown in the first part of the proof of Theorem 19. The Gaussian comparison Theorem 28 yields that\( A_2 \leq C \Delta_{n,3} + \frac{2}{n} \). To bound the term \( A_3 \), we repeat the arguments used in the first part of the proof of Theorem 19, applied to the larger class \( \mathcal{P}_n^* \) and restricting to the event \( \mathcal{E}_n \). As argued above, we will replace \( \psi \) with \( \hat{\psi} \) and \( \hat{\psi}^* \) and, similarly, \( \Gamma \) with \( \hat{\Gamma} \) and \( \hat{\Gamma}^* \). The assumption that \( n \) is large enough guarantees that, with probability at least \( 1 - \frac{2}{n} \), both \( v_n \) and \( \sigma^2_n \) are positive. Thus, the right hand side of (100) serves as an upper bound for the current term \( A_3 \) as well. The claimed bound (72) then follows. \( \Box \)

### 12 Appendix 5: Proofs of Auxiliary Results

**Proof of Lemma 23.** Let \( Z \) be the number of objects that are not selected. Then \( \mathbb{E}[Z] = n \left( 1 - \frac{1}{n} \right)^n \leq \frac{n}{e} \). Next, by the bounded difference inequality,

\[ \mathbb{P}(|Z - \mathbb{E}[Z]| \geq t) \leq 2e^{-\frac{t^2}{2n}}, \]

which implies that

\[ \mathbb{P}(Z > n - d) \leq \exp\left\{ -\frac{(n - d - n(1 - 1/n)^n)^2}{2n} \right\}. \]

The claim (80) follows immediately, since \( n \geq \frac{d}{2} \) and \( (1 - \frac{1}{n})^n \leq e^{-1} \) for all \( n = 1, 2, \ldots \).

\( \Box \)

**Proof of Lemma 24.** Let \( \psi \) be an arbitrary point in \( \mathcal{S}_n \) and \( G = G(\psi) \in \mathbb{R}^{s \times b} \) be the corresponding Jacobian. Recall that, for \( j = 1, \ldots, s \) the \( j \)th row of \( G \) is the transpose of \( G_j = G_j(\psi) \), the gradient of \( g_j \) at \( \psi \). Let\( \mathcal{V} = \mathcal{V}(G) = \{v_1, \ldots, v_{2s}\} \), where for \( j = 1, 2, \ldots, s \), we define \( v_{2j-1} = \frac{G_j}{\|G_j\|} \) and \( v_{2j} = -\frac{G_j}{\|G_j\|} \). For a given \( t > 0 \) and for any Jacobian matrix \( G = G(\psi) \), set

\[ P(G, t) = \left\{ x \in \mathbb{R}^b : v_l^\top x \leq t_l, \forall v_l \in \mathcal{V}(G) \right\}, \tag{101} \]

where, for \( j = 1, \ldots, s \), \( t_{2j-1} = t_{2j} = \frac{1}{\|G_j\|} \).

Recalling that \( \hat{\nu} = G(\hat{\psi}) \), we have that

\[ \|\sqrt{n}(\hat{\nu} - \nu)\|_\infty \leq t \quad \text{if and only if} \quad \sqrt{n}(\hat{\psi} - \psi) \in P(G, t). \]

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Similarly, if \( \tilde{Z}_n \sim N_0(0, V) \) and \( Z_n = G \tilde{Z}_n \sim N_0(\Gamma) \)

\[
\|Z_n\|_\infty \leq t \quad \text{if and only if} \quad \tilde{Z}_n \in P(G, t).
\]

Now consider the class \( \mathcal{A} \) of all subsets of \( \mathbb{R}^b \) of the form specified in (101), where \( t \) ranges over the positive reals and \( G \) ranges in \( \{G(\psi(P)), P \in \mathcal{P}\} \). Notice that this class is comprised of polytopes with at most \( 2s \) facets. Also, from the discussion above,

\[
\sup_{P \in \mathcal{P}, t > 0} \left| \mathbb{P}(\sqrt{n}(\hat{\psi} - \psi) \in A) - \mathbb{P}(\tilde{Z}_n \in A) \right| = \sup_{A \in \mathcal{A}} \left| \mathbb{P}(\sqrt{n}(\hat{\psi} - \psi) \in A) - \mathbb{P}(\tilde{Z}_n \in A) \right|.
\]

(102)

The claimed result follows from applying the Berry-Esseen bound for polyhedral classes, Theorem 27 in the appendix, due to Chernozhukov et al. (2014) to the term on the left hand side of (102). To that end, we need to ensure that conditions (M1'), (M2') and (E1') in that Theorem are satisfied.

For each \( i = 1, \ldots, n \), set \( \tilde{W}_i = (\tilde{W}_{i,1}, \ldots, \tilde{W}_{i,2s}) = (\left( W_i - \psi \right)^\top v, v \in \mathcal{V}(G)) \). Condition (M1') holds since, for each \( l = 1, \ldots, 2s \),

\[
\mathbb{E}\left[ |\tilde{W}_{i,l}|^2 \right] \geq \min_l \mathbb{E}(v_l^\top Vv_l) \geq \lambda_{\text{min}}(V),
\]

where \( V = \text{Cov}[W] \). Turning to condition (M2'), we have that, for each \( l = 1, \ldots, 2s \) and \( k = 1, 2 \),

\[
\begin{align*}
\mathbb{E}\left[ |\tilde{W}_{i,l}|^{2+k} \right] &\leq \mathbb{E}\left[ |v_l^\top (W_i - \psi)|^{2+k} \right] \\
&\leq \mathbb{E}\left[ |v_l^\top (W_i - \psi)|^2 \right] \left( 2A\sqrt{\bar{b}} \right)^k \\
&\leq \bar{v} \left( 2A\sqrt{\bar{b}} \right)^k,
\end{align*}
\]

where the first inequality follows from the bound \( |v_l^\top (W_i - \psi)| \leq \|W_i - \psi\| \) (as each \( v_l \) is of unit norm), the second from the fact that the coordinates of \( W_i \) are bounded in absolute value by \( A \) and the third by the fact that \( \bar{v} \) is the largest eigenvalue of \( V \).

Thus we see that by setting \( B_n = \bar{v} \left( 2A\sqrt{\bar{b}} \right) \), condition (M2') is satisfied (here we have used the fact that \( \bar{v} \geq 1 \)). Finally, condition (E1') is easily satisfied, possibly by increasing the constant in the term \( B_n \).

Thus, Theorem 27 gives

\[
\sup_{A \in \mathcal{A}} \left| \mathbb{P}(\sqrt{n}(\hat{\psi} - \psi) \in A) - \mathbb{P}(\tilde{Z}_n \in A) \right| \leq C \frac{1}{\sqrt{\lambda_{\text{min}}(V)}} \left( \frac{\bar{v}^2b(\log 2bn)^7}{n} \right)^{1/6},
\]

and the result follows from (102), the fact that the choice of \( G = G(\psi) \) is arbitrary and the fact that \( \lambda_{\text{min}}(V(P)) \geq v \) for all \( P \in \mathcal{P}_n \), by assumption. \( \square \)
Lemma 25. Let $X_1, \ldots, X_n$ be independent, mean-zero vectors in $\mathbb{R}^p$, where $p \leq n$, such that $\max_{i=1,\ldots,n} \|X_i\|_\infty \leq K$ almost surely for some $K > 0$ with common covariance matrix $\Sigma$ with $\lambda_{\text{max}}(\Sigma) \leq U$. Then, there exists a universal constant $C > 0$ such that

$$\mathbb{P} \left( \frac{1}{n} \left\| \sum_{i=1}^{n} X_i \right\| \leq CK \sqrt{\frac{\log n}{n}} \right) \geq 1 - \frac{1}{n}. \quad (103)$$

Letting $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} X_i X_i^\top$, if $U \geq \eta > 0$, then there exists a $C > 0$, dependent on $\eta$ only, such that

$$\mathbb{P} \left( \|\hat{\Sigma} - \Sigma\|_{\text{op}} \leq CK \sqrt{\frac{\log p + \log n}{n}} \right) \geq 1 - \frac{1}{n}. \quad (104)$$

Proof of Lemma 25. Since $\|X_i\| \leq K \sqrt{p}$ and $\mathbb{E} \left[ \|X_i\|^2 \right] \leq Up$ for all $i = 1, \ldots, n$, Proposition 1.2 in Hsu et al. (2012) yields that

$$\mathbb{P} \left( \frac{1}{n} \left\| \sum_{i=1}^{n} X_i \right\| \leq \sqrt{U p \frac{n}{n} + \sqrt{8 U p \frac{n}{n} \log n + 4K \sqrt{p} \frac{n}{n} \log n}} \right) \geq 1 - \frac{1}{n}. \quad (105)$$

Equation (103) follows by bounding $\mathbb{E} \left[ \|X_i\|^2 \right]$ with $K^2 p$ instead of $Up$.

Next, we prove (104). We let $\preceq$ denote the positive semi-definite ordering, whereby, for any $p$-dimensional symmetric matrices $A$ and $B$, $A \preceq B$ if and only if $B - A$ is positive semi-definite. For each $i = 1, \ldots, n$, the triangle inequality and the assumptions in the statement yield the bound

$$\left\| X_i X_i^\top - \Sigma \right\|_{\text{op}} \leq \|X_i\|^2 + \lambda_{\text{max}}(\Sigma) \leq K^2 p + U.$$

Similarly, $\mathbb{E} \left[ (X_i X_i^\top)^2 \right] - \Sigma \preceq K^4 p I_p$, with $I_p$ the $p$-dimensional identity matrix. Thus, applying the Matrix Bernstein inequality (see Theorem 1.4 in Tropp, 2012), we obtain that

$$\mathbb{P} \left( \|\hat{\Sigma} - \Sigma\|_{\text{op}} \leq \sqrt{2K^2 p U \frac{\log p + \log 2n}{n} + \frac{2}{3} (K^2 p + U) \frac{\log p + \log 2n}{n}} \right) \geq 1 - \frac{1}{n}. \quad (106)$$

The bound (104) follows from choosing $C$ large enough, depending on $\eta$, and using the fact that $p \leq n$. □

Remark. From (106), by using the looser bounds

$$\left\| X_i X_i^\top - \Sigma \right\|_{\text{op}} \leq 2K^2 p \quad \text{and} \quad \mathbb{E} \left[ (X_i X_i^\top)^2 \right] - \Sigma \preceq K^4 p^2 I_p,$$

one can obtain directly that

$$\mathbb{P} \left( \|\hat{\Sigma} - \Sigma\|_{\text{op}} \leq CK^2 p \sqrt{\frac{\log p + \log n}{n}} \right) \geq 1 - \frac{1}{n}, \quad (107)$$
for some universal constant $C > 0$. Clearly, the scaling in $p$ is worse.

**Proof of Lemma 22.** Throughout, we drop the dependence on $\hat{S}$ in our notation and assume without loss of generality that $\hat{S} = \{1, \ldots, k\}$. We refer the reader to Magnus and Neudecker (2007) for a comprehensive treatment of matrix calculus techniques. Recall that $\psi = \begin{bmatrix} \sigma \\ \alpha \end{bmatrix}$ and $\xi = \begin{bmatrix} w \\ \alpha \end{bmatrix}$, where $\sigma = \text{vec}(\Sigma)$ and $w = \text{vec}(\Omega)$. The dimension of both $\psi$ and $\xi$ is $b = k^2 + k$. For $1 \leq j \leq n$, let

$$
\beta_j = g_j(\psi) = e_j^\top \Omega \alpha,
$$

where $e_j$ is the $j$th elements of the standard basis in $\mathbb{R}^n$. Then, we can write $g_j(\psi) = g(f(\psi))$, with $f(\psi) = \xi \in \mathbb{R}^b$ and $g(\xi) = e_j^\top \Omega \alpha \in \mathbb{R}$.

Using the chain rule, the derivative of $g_j(\psi)$ is

$$
Dg_j(\psi) = Dg(\xi)Df(\psi) = e_j^\top \left( \left( \alpha^\top \otimes I_k \right) E + \Omega F \right)
$$

where

$$
E = \begin{bmatrix} I_{k^2} & 0_{k^2 \times k} \end{bmatrix} \in \mathbb{R}^{k^2 \times b} \quad \text{and} \quad F = \begin{bmatrix} 0_{k \times k^2} & I_k \end{bmatrix} = \frac{d\alpha}{d\psi} \in \mathbb{R}^{k \times b}.
$$

Carrying out the calculations, we have that

$$
\left( \alpha^\top \otimes I_k \right) E \begin{bmatrix} -\Omega \otimes \Omega & 0 \\ 0 & I_k \end{bmatrix} = \left( \alpha^\top \otimes I_k \right) \begin{bmatrix} I_{k^2} & 0_{k^2 \times k} \end{bmatrix} \begin{bmatrix} -\Omega \otimes \Omega & 0 \\ 0 & I_k \end{bmatrix}
$$

$$
= \left( -\alpha^\top \otimes I_k \right) \begin{bmatrix} \Omega \otimes \Omega & 0 \\ 0 & I_k \end{bmatrix}
$$

and

$$
\Omega F \begin{bmatrix} -\Omega \otimes \Omega & 0 \\ 0 & I_k \end{bmatrix} = \Omega \begin{bmatrix} 0_{k \times k^2} & I_k \end{bmatrix} \begin{bmatrix} -\Omega \otimes \Omega & 0 \\ 0 & I_k \end{bmatrix}
$$

$$
= \Omega \begin{bmatrix} 0_{k \times k^2} & I_k \end{bmatrix} = \begin{bmatrix} 0_{k \times k^2} & \Omega \end{bmatrix}.
$$

Plugging the last two expressions into the initial formula for $Dg_j(\psi)$ we obtain that

$$
Dg_j(\psi) = e_j^\top \left( \left[ -\left( \alpha^\top \otimes I_k \right) (\Omega \otimes \Omega) 0_{k \times k^2} \right] + [0_{k \times k^2} \Omega] \right)
$$

$$
= e_j^\top \left( \left[ -\left( \alpha^\top \otimes I_k \right) (\Omega \otimes \Omega) \Omega \right] \right).
$$

(108)

The gradient of $g_j$ at $\psi$ is just the transpose of $Dg_j(\psi)$. Thus, the Jacobian of the function $g$ is

$$
\beta_j/d\psi = G = \begin{pmatrix} G_1^\top \\
\vdots \\
G_k^\top \end{pmatrix}.
$$

(109)
Next, we compute $Hg_j(\psi)$, the $b \times b$ Hessian of $g_j$ at $\psi$. Using the chain rule,

$$Hg_j(\psi) = D(Dg_j(\psi)) = (I_b \otimes e_j^T) \frac{d}{d\psi} \left[ \frac{d}{d\psi} \begin{pmatrix} \begin{bmatrix} (\alpha^T \otimes I_k) (\Omega \otimes \Omega) & \Omega \end{bmatrix} \end{pmatrix} \right],$$

where the first matrix is of dimension $b \times kb$ and the second matrix is of dimension $kb \times b$. Then,

$$\frac{d}{d\psi} \begin{pmatrix} \begin{bmatrix} (\alpha^T \otimes I_k) (\Omega \otimes \Omega) & \Omega \end{bmatrix} \end{pmatrix} = \begin{bmatrix} -\frac{d}{d\psi} (\alpha^T \otimes I_k)(\Omega \otimes \Omega) & \frac{d}{d\psi} \Omega \end{bmatrix}.$$  \hfill (110)

The derivative at the bottom of the previous expression is

$$\frac{d\Omega}{d\psi} = \frac{d\Omega}{d\Sigma} \frac{d\Sigma}{d\psi} = -(\Omega \otimes \Omega)E = -(\Omega \otimes \Omega)[I_{k^2} \quad 0_{k^2 \times k}] = \begin{bmatrix} - (\Omega \otimes \Omega) & 0_{k^2 \times k} \end{bmatrix}.$$  

The top derivative in (110) is more involved. By the product rule,

$$\frac{d}{d\psi} \left( (\Omega \otimes \Omega) (\Omega \otimes \Omega) \right) = \left( (\Omega \otimes \Omega) (\Omega \otimes \Omega) + (\Omega \otimes \Omega) \right) \frac{d}{d\psi} \begin{bmatrix} (\alpha^T \otimes I_k) \frac{d}{d\psi} \begin{bmatrix} (\alpha^T \otimes I_k)(\Omega \otimes \Omega) & \Omega \end{bmatrix} \end{bmatrix} + \begin{bmatrix} (I_{k^2} \otimes (\alpha^T \otimes I_k)) \frac{d}{d\psi} \begin{bmatrix} (\Omega \otimes \Omega) \end{bmatrix} \end{bmatrix}.$$  

The first derivative in the last expression is

$$\frac{d}{d\psi} \left( (\Omega \otimes \Omega) \right) = \frac{d}{d\psi} \begin{bmatrix} (\Omega \otimes \Omega) \end{bmatrix} = \begin{bmatrix} 0_{k^2 \times k^2} & I_k \end{bmatrix},$$

where $K_{k,1}$ is the appropriate commutation matrix and the third identity follows since $K_{k,1} = I_k$ and, therefore, $(I_k \otimes K_{1,k} \otimes I_k) = I_{k^3}$. Continuing with the second derivative in (110),

$$\frac{d}{d\psi} \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} = \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} \frac{d}{d\psi} \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} = -J(\Omega \otimes \Omega)E$$

where

$$J = \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} \begin{bmatrix} (I_k \otimes K_{k,k} \otimes I_k) \end{bmatrix} (I_{k^2} \otimes \text{vec}(I_k)) + \begin{bmatrix} (I_k \otimes \Omega, \Omega, I_k) \end{bmatrix} \begin{bmatrix} (I_k \otimes K_{k,k} \otimes I_k) \end{bmatrix} \begin{bmatrix} (\text{vec}(I_k) \otimes I_{k^2}) \end{bmatrix}.$$  

To see this, notice that, by the product rule, we have

$$J = \frac{d}{d\Omega} \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} = \frac{d}{d\Omega} \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} (I_{k^2} \otimes \text{vec}(I_k)) + \begin{bmatrix} (I_k \otimes \Omega, \Omega, I_k) \end{bmatrix} \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} \frac{d}{d\Omega} \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix}.$$  

Next,

$$\frac{d}{d\Omega} \begin{bmatrix} (I_k \otimes \Omega, \Omega) \end{bmatrix} = \begin{bmatrix} (I_k \otimes K_{k,k} \otimes I_k) \end{bmatrix} \begin{bmatrix} (I_{k^2} \otimes \text{vec}(I_k)) \end{bmatrix} = \begin{bmatrix} (I_k \otimes K_{k,k}) \end{bmatrix} \begin{bmatrix} (I_k \otimes \text{vec}(I_k) \otimes I_k) \end{bmatrix}.$$  

65
and
\[\frac{d(I_k \otimes \Omega)}{d\Omega} = (I_k \otimes K_{k,k} \otimes I_k)\left(\text{vec}(I_k) \otimes I_{k^2}\right) = (K_{k,k} \otimes I_{k^2})\left(I_k \otimes \text{vec}(I_k) \otimes I_k\right).\]

The formula for \(J\) follows from the last three expressions. Notice that \(J\) is matrix of size \(k^4 \times k^2\).

Finally, plugging the expressions for \(d(\alpha^\top \otimes I_k)(\Omega \otimes \Omega)\) and \(\frac{d\Omega}{d\psi}\) in (110) we get that the Hessian \(Hg_j(\psi)\) is
\[
\frac{1}{2} \left( (I_b \otimes e_j^\top)H + H^\top (I_b \otimes e_j) \right)
\]
where
\[
H = \begin{bmatrix}
-((\Omega \otimes \Omega) \otimes I_k) & 0_{k^3 \times k^2} & I_k \otimes \text{vec}(I_k) + (I_{k^2} \otimes (\alpha^\top \otimes I_k))J\begin{bmatrix} \Omega \otimes \Omega & 0_{k^2 \times k} \end{bmatrix} \\
-\Omega \otimes \Omega & 0_{k^2 \times k}
\end{bmatrix}
\]
(112)

So far we have ignored the facts that \(\Sigma\) is symmetric. Account for the symmetry, the Hessian of \(g_j(\psi)\) is
\[
D_h^\top Hg_j(\psi)D_h,
\]
where \(D_h\) is the modified duplication matrix such that \(D\psi_h = \psi\), with \(\psi_h\) the vector comprised by the sub-vector of \(\psi\) not including the entries corresponding to the upper (or lower) diagonal entries of \(\Sigma\).

We now prove the bounds (78) and (79). We will use repeatedly the fact that \(\sigma_1(A \otimes B) = \sigma_1(A)\sigma_1(B)\) and, for a vector \(x\), \(\sigma_1(x) = \|x\|\). For notational convenience, we drop the dependence on \(\psi\), since all our bounds hold uniformly over all \(\psi \in S_n\). The first bound in (78) on the norm of the gradient of \(g_j\) is straightforward:

\[
\|G_j\| \leq \|e_j\| \times \sigma_1\left(-\left(\begin{bmatrix} \Omega \otimes \Omega \end{bmatrix}\right)\right) \\
\leq \left(\|\alpha\| \times \sigma_1(\Omega)^2 + \sigma_1(\Omega)\right) \\
\leq \frac{A^2\sqrt{k}}{u^2} + \frac{1}{u} \\
\leq C\frac{\sqrt{k}}{u^2},
\]
(113)
since \(\sigma_1(\Omega) \leq \frac{1}{u}, \|\alpha\| \leq \sqrt{A^2\text{tr}(\Sigma)} \leq A^2\sqrt{k}\), and we assume that \(k \geq u^2\).

Turning to the second bound in (78), we will bound the largest singular values of the individual terms in (111). First, for the lower block matrix in (112), we have that
\[
\sigma_1(\begin{bmatrix} \Omega \otimes \Omega & 0_{k^2 \times k} \end{bmatrix}) = \sigma_1(\begin{bmatrix} \Omega \otimes \Omega \end{bmatrix}) = \sigma_1^2(\Omega) = 1/u^2.
\]
Next, we consider the two matrices in the upper block part of (112). For the first matrix we have that

$$\sigma_1 \left( (\Omega \otimes \Omega \otimes I_k) \begin{bmatrix} 0_{k^3 \times k^2} & I_k \otimes \text{vec}(I_k) \end{bmatrix} \right) = \sigma_1 \left( \begin{bmatrix} 0_{k^3 \times k^2} & \Omega \otimes \text{vec}(\Omega) \end{bmatrix} \right)$$

$$= \sigma_1 (\Omega \otimes \text{vec}(\Omega))$$

$$= \sigma_1(\Omega)\sigma_1(\text{vec}(\Omega))$$

$$\leq \sqrt{k} u^2,$$

since

$$\sigma_1(\text{vec}(\Omega)) = ||\Omega||_F = \sqrt{\sum_{i=1}^{k} \sigma_i^2(\Omega)} \leq \sqrt{k}\sigma_1(\Omega) = \frac{\sqrt{k}}{u}.$$

The identity in (114) is established using the following facts, valid for conformal matrices $A$, $B$, $C$, $D$ and $X$:

- $(A \otimes B)(C \otimes D) = AC \otimes BD$, with $A = \Omega$, $B = \Omega \otimes I_k$, $C = I_k$ and $D = \text{vec}(\Omega)$, and
- $AXB = C$ is equivalent to $(B^\top \otimes A) \text{vec}(X) = \text{vec}(C)$, with $B = C = \Omega$ and $X = A = I_k$.

We now bound \(\sigma_1 \left( [I_{k^2} \otimes \alpha^\top \otimes I_k] J [\Omega \otimes \Omega \otimes 0_{k^2 \times k}] \right)\), the second matrix in the upper block in (112). We have that

$$\sigma_1(J) \leq 2\sigma_1((I_k \otimes \Omega \otimes I_{k^2})(I_k \otimes K_{k,k} \otimes I_k)(I_{k^2} \otimes \text{vec}(I_k)))$$

$$= 2\sigma_1(\Omega)||I_k||_F$$

$$= 2\sqrt{k}\sigma_1(\Omega),$$

since $\sigma_1(K_{k,k}) = 1$. Hence, using the fact that $\sigma_1([I_{k^2} \otimes \alpha^\top \otimes I_k]) = ||\alpha||$,

$$\sigma_1 \left( [I_{k^2} \otimes \alpha^\top \otimes I_k] J [\Omega \otimes \Omega \otimes 0_{k^2 \times k}] \right) \leq 2\sqrt{k}||\alpha||\sigma_1^2(\Omega) \leq 2\sqrt{AUk} \frac{k}{u^3},$$

since $||\alpha|| \leq \sqrt{AUk}$. Thus, we have obtained the following bound for the largest singular value of the matrix $H$ in (112):

$$\sigma_1(H) \leq C \left( \frac{1}{u^2} + \frac{\sqrt{k}}{u^2} + \frac{k}{u^3} \right),$$

where $C$ is a positive number depending on $A$ only. Putting all the pieces together,

$$\sigma_1(H_j) = \sigma_1 \left( \frac{1}{2}((I_b \otimes e_j)H + H^\top(I_b \otimes e_j)) \right)$$

$$\leq \sigma_1((I_b \otimes e_j)H)$$

$$\leq \sigma_1(I_b)\sigma_1(e_j)\sigma_1(H)$$

$$\leq C \left( \frac{1}{u^2} + \frac{\sqrt{k}}{u^2} + \frac{k}{u^3} \right).$$
Whenever \( u \leq \sqrt{k} \), the dominant term in the above expression is \( \frac{k}{u^m} \). This gives the bound on \( \overline{H} \) in (78). The bound on \( \overline{\sigma} \) given in (79) follows from (76). Indeed, for every \( P \in P_{\text{OLS}} \)

\[
\min_j \sqrt{G_j V G_j^\top} \geq \sqrt{v} \min_j \|G_j\|.
\]

Then, using (76),

\[
\min_j \|G_j\| \geq \min_j \|\Omega_j\| \geq \lambda_{\min}(\Omega) = \frac{1}{U},
\]

where \( \Omega_j \) denotes the \( j \)th row of \( \Omega \).

The final value of the constant \( C \) depends only on \( A \) and \( U \), and since \( U \leq A \), we can reduce the dependence of such constant on \( A \) only.

□

13 Appendix 6: Anti-concentration and comparison bounds for maxima of Gaussian random vectors and Berry-Esseen bounds for polyhedral sets

Now we collect some results that can be are derived from Chernozhukov et al. (2015), Chernozhukov et al. (2014) and Nazarov (2003). However, our statement of the results is slightly different than in the original papers. The reason for this is that we need to keep track of some constants in the proofs that affect our rates.

The following anti-concentration result for the maxima of Gaussian vectors follows from Lemma A.1 in Chernozhukov et al. (2014) and relies on a deep result in Nazarov (2003).

**Theorem 26** (Anti-concentration of Gaussian maxima). Let \((X_1, \ldots, X_p)\) be a centered Gaussian vector in \( \mathbb{R}^p \) with \( \sigma_j^2 = \mathbb{E}[X_j^2] > 0 \) for all \( j = 1, \ldots, p \). Moreover, let \( \overline{\sigma} = \min_{1 \leq j \leq p} \sigma_j \). Then, for any \( y = (y_1, \ldots, y_p) \in \mathbb{R}^p \) and \( a > 0 \)

\[
\mathbb{P}(X_j \leq y_j + a, \forall j) - \mathbb{P}(X_j \leq y_j, \forall j) \leq \frac{a}{\overline{\sigma}} \left( \sqrt{2 \log p + 2} \right).
\]

The previous result implies that, for any \( a > 0 \) and \( y = (y_1, \ldots, y_p) \in \mathbb{R}^p_+ \),

\[
\mathbb{P}(\max_j |X_j| \leq y_j + a, \forall j) - \mathbb{P}(\max_j |X_j| \leq y_j, \forall j) \leq \frac{a}{\overline{\sigma}} \left( \sqrt{2 \log 2p + 2} \right)
\]

and that, for any \( y > 0 \),

\[
\mathbb{P}(\max_j |X_j| \leq y + a) - \mathbb{P}(\max_j |X_j| \leq y) \leq \frac{a}{\overline{\sigma}} \left( \sqrt{2 \log 2p + 2} \right).
\]
The following high-dimensional central limit theorem follows from Proposition 2.1 in Chernozhukov et al. (2014) and Theorem 26. Notice that we have kept the dependence on the minimal variance explicit.

**Theorem 27** (Berry-Esseen bound for simple convex sets). Let $X_1, \ldots, X_n$ be independent centered random vectors in $\mathbb{R}^p$. Let $S^X_n = \frac{1}{\sqrt{n}} \sum_{i=1}^n X_i$ and, similarly, let $S^Y_n = \frac{1}{n} \sum_{i=1}^n Y_i$, where $Y_1, \ldots, Y_n$ are independent vectors with $Y_i \sim N_p(0, \mathbb{E}[X_iX_i^\top])$. Let $A$ be the collection of polyhedra $A$ in $\mathbb{R}^p$ of the form

$$A = \left\{ x \in \mathbb{R}^d : v^\top x \leq t_v, v \in \mathcal{V}(A) \right\}$$

where $\mathcal{V}(A) \subset \mathbb{R}^p$ is a set of $m$ points of unit norm, with $m \leq (np)^d$ for some constant $d > 0$, and $(t_v : v \in \mathcal{V}(A))$ is a set of $m$ positive numbers. For each $i = 1, \ldots, n$ let

$$\tilde{X}_i = (\tilde{X}_{i1}, \ldots, \tilde{X}_{im})^\top = \left( v^\top X_i, v \in \mathcal{V}(A) \right).$$

Assume that the following conditions are satisfied, for some $B_n \geq 1$ and $\sigma > 0$:

(M1') $n^{-1} \sum_{i=1}^n \mathbb{E} \left[ \tilde{X}_{ij}^2 \right] \geq \sigma^2$, for all $j = 1, \ldots, m$;

(M2') $n^{-1} \sum_{i=1}^n \mathbb{E} \left[ |\tilde{X}_{ij}|^{2+k} \right] \leq B_n^k$, for all $j = 1, \ldots, m$ and $k = 1, 2$;

(E1') $\mathbb{E} \left[ \exp \left( |\tilde{X}_{i,j}|/B_n \right) \right] \leq 2$, for $i = 1, \ldots, n$ and $k = 1, 2$.

Then, there exists a constant $C > 0$ depending only on $d$ such that

$$\sup_{A \in \mathcal{A}} \left| \mathbb{P}(S^X_n \in A) - \mathbb{P}(S^Y_n \in A) \right| \leq C \frac{\sigma}{2} \left( \frac{B_n^2 \log^7(pn)}{n} \right)^{1/6}.$$

Finally, we make frequent use the following comparison theorem for the maxima of Gaussian vectors. Its proof can be established using arguments from the proof of Theorem 4.1 in Chernozhukov et al. (2014) – which itself relies on a modification of Theorem 1 from Chernozhukov et al. (2015) – along with the above anti-concentration bound of Theorem 26. As usual, we have kept the dependence on the minimal variance explicit.

**Theorem 28** (Gaussian comparison). Let $X \sim N_p(0, \Sigma_X)$ and $Y \sim N_p(0, \Sigma_Y)$ with

$$\Delta = \max_{i,j} |\Sigma_X(j,k) - \Sigma_Y(j,k)|$$

Let $\sigma^2 = \max \{ \min_j \Sigma_X(j,j), \min_j \Sigma_Y(j,j) \}$. Then, there exists a universal constant $C > 0$ such that

$$\sup_{t \in \mathbb{R}^p} |\mathbb{P}(X \leq t) - \mathbb{P}(Y \leq t)| \leq C \frac{\Delta^{1/3}(2 \log p)^{1/3}}{\sigma^{2/3}}.$$
Remark. The above result further implies that
\[
\sup_{t>0} |\mathbb{P}(\|X\|_\infty \leq t) - \mathbb{P}(\|Y\|_\infty \leq t)| \leq 2C \frac{\Delta^{1/3}(2 \log p)^{1/3}}{\sigma^{2/3}},
\]
which corresponds to the original formulation of the Gaussian comparison theorem of Chernozhukov et al. (2015).

14 Appendix 7: The Procedures
Boot-Split

INPUT: Data \( D = \{(X_1, Y_1), \ldots, (X_{2n}, Y_{2n})\} \). Confidence parameter \( \alpha \). Constant \( \epsilon \) (Section 2.2).

OUTPUT: Confidence set \( \hat{C}_S^* \) for \( \beta_S \) and \( \hat{D}_S^* \) for \( \gamma_S \).

1. Randomly split the data into two halves \( D_{1,n} \) and \( D_{2,n} \).
2. Use \( D_{1,n} \) to select a subset of variables \( \hat{S} \). This can be forward stepwise, the lasso, or any other method. Let \( k = |\hat{S}| \).
3. Write \( D_{2,n} = \{(X_1, Y_1), \ldots, (X_n, Y_n)\} \). Let \( P_n \) be the empirical distribution of \( D_{2,n} \).

4. For \( \beta_S \):
   (a) Get \( \hat{\beta}_S \) from \( D_{2,n} \) by least squares.
      i. Draw \( (X_1^*, Y_1^*), \ldots, (X_m^*, Y_m^*) \sim P_n \). Let \( \hat{\beta}_S^* \) be the estimator constructed from the bootstrap sample.
      ii. Repeat \( B \) times to get \( \hat{\beta}_S^*, \ldots, \hat{\beta}_S^{*,B} \).
      iii. Define \( \hat{t}_\alpha \) by
           \[
           \frac{1}{B} \sum_{b=1}^{B} I\left( \sqrt{n}||\hat{\beta}_S^* - \hat{\beta}_S||_\infty > \hat{t}_\alpha \right) = \alpha.
           \]
   (b) Output: \( \hat{C}_S^* = \{\beta \in \mathbb{R}^k : ||\beta - \hat{\beta}_S||_\infty \leq \hat{t}_\alpha/\sqrt{n}\} \).

5. For \( \gamma_S \):
   (a) Get \( \hat{\beta}_S \) from \( D_{1,n} \). This can be any estimator. For \( j \in \hat{S} \) let \( \hat{\gamma}_S(j) = \frac{1}{n} \sum_{i=1}^{n} r_i \) where \( r_i = (\delta_i(j) + \xi_i(j)), \delta_i(j) = |Y_i - \hat{\beta}_S^T X_i| - |Y_i - \hat{\beta}_S^T X_i| \) and \( \xi_i(j) \sim \text{Unif}(-1, 1) \). Let \( \hat{\gamma}_S = (\hat{\gamma}_S(j) : j \in \hat{S}) \).
      i. Draw \( (X_1^*, Y_1^*), \ldots, (X_n^*, Y_n^*) \sim P_n \).
      ii. Let \( \hat{\gamma}_S(j) = \frac{1}{n} \sum_{i=1}^{n} r_i^* \). Let \( \hat{\gamma}_S = (\hat{\gamma}_S^*(j) : j \in \hat{S}) \).
      iii. Repeat \( B \) times to get \( \hat{\gamma}_S^{*,1}, \ldots, \hat{\gamma}_S^{*,B} \).
      iv. Define \( \hat{u}_\alpha \) by
           \[
           \frac{1}{B} \sum_{b=1}^{B} I\left( \sqrt{n}||\hat{\gamma}_S^* - \hat{\gamma}_S||_\infty > \hat{u}_\alpha \right) = \alpha.
           \]
   (b) Output: \( \hat{D}_S^* = \{\gamma \in \mathbb{R}^k : ||\gamma - \hat{\gamma}_S||_\infty \leq \hat{u}_\alpha/\sqrt{n}\} \).

Figure 4: The Boot-Split Algorithm.
Normal-Split

INPUT: Data $\mathcal{D} = \{(X_1, Y_1), \ldots, (X_{2n}, Y_{2n})\}$. Confidence parameter $\alpha$. Threshold and variance parameters $\tau$ and $\epsilon$ (only for $\gamma_{\tilde{S}}$).

OUTPUT: Confidence set $\hat{C}_{\tilde{S}}$ for $\beta_{\tilde{S}}$ and $\hat{D}_{\tilde{S}}$ for $\gamma_{\tilde{S}}$.

1. Randomly split the data into two halves $\mathcal{D}_{1,n}$ and $\mathcal{D}_{2,n}$.
2. Use $\mathcal{D}_{1,n}$ to select a subset of variables $\tilde{S}$. This can be forward stepwise, the lasso, or any other method. Let $k = |\tilde{S}|$.
3. For $\beta_{\tilde{S}}$:
   (a) Get $\hat{\beta}_{\tilde{S}}$ from $\mathcal{D}_{2,n}$ by least squares.
   (b) Output $\hat{C}_{\tilde{S}} = \bigotimes_{j \in \tilde{S}} C(j)$ where $C(j) = \hat{\beta}_{\tilde{S}}(j) \pm z_{\alpha/(2k)} \sqrt{\hat{\Gamma}_n(j,j)}$ where $\hat{\Gamma}$ is given by (16).
4. For $\gamma_{\tilde{S}}$:
   (a) Get $\hat{\beta}_{\tilde{S}}$ from $\mathcal{D}_{1,n}$. This can be any estimator. For $j \in \tilde{S}$ let $\hat{\gamma}_{\tilde{S}}(j) = \frac{1}{n} \sum_{i=1}^{n} r_i$ where $r_i = (\delta_i(j) + \xi_i(j))$, $\delta_i(j) = |Y_i - t_{\tau} \left( \hat{\beta}_{\tilde{S}}^\top X_i \right) | - |Y_i - t_{\tau} \left( \hat{\beta}_{\tilde{S}}^\top X_i \right) |$ and $\xi_i(j) \sim \text{Unif}(-1,1)$. Let $\hat{\gamma}_{\tilde{S}} = (\hat{\gamma}_{\tilde{S}}(j) : j \in \tilde{S})$.
   (b) Output $\hat{D}_{\tilde{S}} = \bigotimes_{j \in \tilde{S}} D(j)$ where $D(j) = \hat{\gamma}_{\tilde{S}}(j) \pm z_{\alpha/(2k)} \hat{\Sigma}(j,j)$, with $\hat{\Sigma}(j,j)$ given by (28).

Figure 5: The Normal-Split Algorithm.
Median-Split

**INPUT:** Data $\mathcal{D} = \{(X_1, Y_1), \ldots, (X_{2n}, Y_{2n})\}$. Confidence parameter $\alpha$.

**OUTPUT:** Confidence set $\hat{E}_S$.

1. Randomly split the data into two halves $\mathcal{D}_{1,n}$ and $\mathcal{D}_{2,n}$.
2. Use $\mathcal{D}_{1,n}$ to select a subset of variables $\hat{S}$. This can be forward stepwise, the lasso, or any other method. Let $k = |\hat{S}|$.
3. Write $\mathcal{D}_{2,n} = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$. For $(X_i, Y_i) \in \mathcal{D}_{2,n}$ let

   $$W_i(j) = |Y_i - \hat{\beta}_{\hat{S},j}^\top X_i| - |Y_i - \hat{\beta}_S^\top X_i|,$$

4. Let $W_{(1)}(j) \leq \cdots \leq W_{(n)}(j)$ be the order statistics and let $E(j) = [W_{(n-k_2)}, W_{(n-k_1+1)}]$ where

   $$k_1 = \frac{n}{2} + \sqrt{n \log \left(\frac{2k}{\alpha}\right)}, \quad k_2 = \frac{n}{2} - \sqrt{n \log \left(\frac{2k}{\alpha}\right)}.$$

5. Let $\hat{E}_S = \bigotimes_{j \in S} E(j)$.

Figure 6: The Median-Split Algorithm.