A Power Analysis for Knockoffs with the Lasso Coefficient-Difference Statistic

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Abstract

In a linear model with possibly many predictors, we consider variable selection procedures given by
\[ \{1 \leq j \leq p : |\hat{\beta}_j(\lambda)| > t\}, \]
where \( \hat{\beta}(\lambda) \) is the Lasso estimate of the regression coefficients, and where \( \lambda \) and \( t \) may be data dependent. Ordinary Lasso selection is captured by using \( t = 0 \), thus allowing to control only \( \lambda \), whereas thresholded-Lasso selection allows to control both \( \lambda \) and \( t \). The potential advantages of the latter over the former in terms of power—figuratively, opening up the possibility to look further down the Lasso path—have been quantified recently leveraging advances in approximate message-passing (AMP) theory, but the implications are actionable only when assuming substantial knowledge of the underlying signal.

In this work we study theoretically the power of a knockoffs-calibrated counterpart of thresholded-Lasso that enables us to control FDR in the realistic situation where no prior information about the signal is available. Although the basic AMP framework remains the same, our analysis requires a significant technical extension of existing theory in order to handle the pairing between original variables and their knockoffs. Relying on this extension we obtain exact asymptotic predictions for the true positive proportion achievable at a prescribed type I error level. In particular, we show that the knockoffs version of thresholded-Lasso can perform much better than ordinary Lasso selection if \( \lambda \) is chosen by cross-validation on the augmented matrix.

1 Introduction

Suppose that we observe a matrix \( X \in \mathbb{R}^{n \times p} \) of predictor measurements and a response vector \( Y \in \mathbb{R}^n \), and assume that
\[ Y = X\beta + \xi, \quad \xi \sim \mathcal{N}_n(0, \sigma^2 I), \]
where \( \beta = (\beta_1, ..., \beta_p)^\top \) and \( \sigma^2 \) are unknown. In many modern applications where the linear model is appropriate, \( p \) is large and we may have a reason to believe a priori that \( \beta_j \) is small in magnitude for most \( j = 1, ..., p \). For example, in genetics \( X_{ij} \) might encode the state (presence or absence)
of a specific genetic variant $j$ for individual $i$, and $Y_i$ measures a quantitative trait of interest. Typical cases entail the number $p$ of genetic variants in the millions but, for all we know about this kind of problems, only a small number of them are highly explanatory for the response. Finding mutations which are in that sense important among the $p$ candidates, is key to investigating the causal mechanism regulating the trait.

1.1 Controlled variable selection

We treat the problem formally as a multiple hypothesis testing problem with respect to the model (1.1), where the null hypotheses to be tested are

$$H_0^j : \beta_j = 0, \quad j \in \mathcal{H} \equiv \{1, \ldots, p\}.$$ 

Denote by $\mathcal{H}_0 \equiv \{j : \beta_j = 0\}$ the (unknown) subset of nulls, and denote by $\mathcal{S} \equiv \mathcal{H} \setminus \mathcal{H}_0$ the subset of nonnulls. In general, a test uses the data to output an estimate $\hat{S} \subseteq \{1, \ldots, p\}$ of $\mathcal{S}$. Define the false positive proportion and the true positive proportion as

$$\text{FDP} \equiv \frac{|\hat{S} \cap \mathcal{H}_0|}{|\hat{S}|} \quad \text{and} \quad \text{TPP} \equiv \frac{|\hat{S} \cap \mathcal{S}|}{|\mathcal{S}|},$$

respectively, with the convention $0/0 \equiv 0$. A good test is one for which TPP is large and FDP is small, meaning that the test is able to separate nonnulls from nulls. We will later be concerned with the concrete problem of controlling the false discovery rate, $\text{FDR} \equiv \mathbb{E}[\text{FDP}]$, below a prespecified level, and we say that a test is valid at level $q$ if $\text{FDR} \leq q$ for all $\beta$. Before proceeding we note that, per definition, any variable selection procedure is a legitimate test and vice versa, and we will use the two terms interchangeably.

With a growing interest in high-dimensional (large $p$) settings, considerable attention has been given over the past two decades to variable selection procedures relying on the Lasso program,

$$\text{minimize}_{b \in \mathbb{R}^p} \frac{1}{2} \|Y - Xb\|_2^2 + \lambda \|b\|_1.$$  

(1.2)

The Lasso program is appealing because it is relatively easy to solve and at the same time the solution to (1.2), call it $\hat{\beta}(\lambda)$, tends to be sparse. Thus, variable selection is readily elicited by associating with $\hat{\beta}(\lambda)$ the subset

$$\hat{\mathcal{S}} \equiv \{j : |\hat{\beta}_j(\lambda)| \neq 0\}. \quad \text{(1.3)}$$

Indeed, many works have studied the properties of this selection procedure, mostly establishing conditions on $X$ and $\beta$ for selection consistency, $\mathbb{P}(\hat{\mathcal{S}} = \mathcal{S}) \to 1$, e.g. [13, 24, 26, 19, 6, 11]. Such conditions turn out to be generally very stringent even in the noiseless case, $\sigma^2 = 0$; in other words, the fundamental phenomenon is not a matter of insufficient signal-to-noise ratio. While the conditions for (1.3) to recover a superset of the true support $\mathcal{S}$, also referred to as screening, are considerably less restrictive, it tends to select too many null variables (see, e.g., [23, 6, 25]). This rather discouraging fact has motivated practitioners and theoreticians alike to consider post-processing of the solution to (1.2). The simplest and perhaps most notable such procedure sets

$$\hat{\mathcal{S}} \equiv \{j : |\hat{\beta}_j(\lambda)| > t\}, \quad \text{(1.4)}$$
where \( t > 0 \) is fixed or data-dependent. Hence, we now have two different variable selection procedures deriving from the Lasso program:

- **Lasso**: this is the procedure given by (1.3).
- **Thresholded-Lasso**: this is the procedure given by (1.4).

This paper is about a precise quantitative comparison of the relative merits of these two procedures.

1.2 “Vertical” look at the Lasso path

At first glance, the two selection rules might not appear that different, because (1.3) is just (1.4) with \( t = 0 \). There is, however, a fundamental difference between Lasso and thresholded-Lasso. To illustrate this, we simulated data from the model with \( n = 100, p = 200, \sigma = 1 \), and the coefficients are all zero except for \( \beta_1 = \ldots = \beta_{20} = 10 \). Figure 1 tracks the absolute value of the Lasso estimates \( \hat{\beta}_j(\lambda) \) as \( \lambda \) varies, for null coefficients and for nonnull coefficients. We can see that false discoveries occur early on the Lasso path (as already observed in [15]). Consequently, (1.3) cannot keep FDP small unless \( \lambda \) is chosen large, which inevitably affects the power: in this example the maximum TPP for (1.3) subject to FDP \( \leq 0.1 \) is 0.45. Nevertheless, it is also evident from the figure that the estimates corresponding to true signals maintain significantly larger size than most of the estimates for nulls, as \( \lambda \) decreases. The additional flexibility in varying the threshold allows (1.4) to take advantage of this: basically, \( \lambda \) can be chosen freely, while setting \( t \) appropriately large will make FDP small (by killing small estimates corresponding to null coefficients). Figuratively, Lasso (1.3) looks at the path “horizontally”—see discussion in the beginning of Subsection 2.2—and so it is committed to the order in which variables enter one after the other; whereas thresholded-Lasso (1.4) looks at the path “vertically”, exploiting the extra degree of freedom to specify \( t \). That the latter can be advantageous is shown in the figure by the broken line, indicating the 10-fold cross-validation estimate of \( \lambda \). At this value of \( \lambda \), for example, thresholded-Lasso has TPP equal to 0.95 when \( t \) is selected such that FDP \( \leq 0.1 \).

We are certainly not the first to observe that taking the magnitude of the coefficient estimate into account can improve dramatically the separation between nulls and nonnulls; this phenomenon is studied in [25, 23, 7, 16], among others. It was recent developments in approximate message-passing (AMP) theory, however, that enabled a precise theoretical comparison between Lasso and thresholded-Lasso under the error metrics defined above, if only in a particular setup. Thus, in a special case where \( X \) has i.i.d. Gaussian entries, and in the asymptotic regime where \( p \) is comparable to \( n \), and the sparsity is linear, \( |\mathbb{S}| \approx c p \), [5] leveraged results from [4] to first obtain exact asymptotic predictions of FDP and TPP for Lasso. A fundamental quantitative tradeoff between FDP and TPP for Lasso, valid uniformly in \( \lambda \), was presented in [15], implying in particular that Lasso cannot achieve exact support recovery in the above setting. More recently, [21] extended the results of [15] to obtain predictions of FDP and TPP for thresholded-Lasso (and even more generally, for bridge estimators). The results of [16] imply further that in this asymptotic setting, thresholded-Lasso recovers the true model if the limiting signal sparsity is below the transition curve of [10] and the magnitude of the nonzero \( \beta_j \) diverges to infinity.

1.3 Our contribution

The works of [15] and [21] are important because they facilitate a theoretical yet precise comparison between Lasso and thresholded-Lasso. However, in practice the implications are limited: the calcu-
lations in both papers will yield the achievable asymptotic FDP for a prescribed asymptotic TPP level at any given $\lambda$ for (1.3) and at any given $t$ for (1.4), provided that $\sigma$ and the empirical distribution of the true coefficients $\beta_j$ are known. In reality, such a-priori knowledge about the signal and the noise level is rarely available. This realization motivated [22] to study a knockoffs-augmented setup and obtain an operable counterpart to the “oracle” FDP-TPP curve of [15] for Lasso. By “operable” we mean that the power predictions of [22] apply to a procedure that provably controls the FDR without any knowledge about $\beta$ or $\sigma$.

In the present article we obtain an operable analog to the FDP and TPP predictions of [21] for thresholded-Lasso. As in [22], we employ knockoffs to allow for FDR calibration, the basic idea being that the augmented setup can be studied within the same AMP framework. However, there is a crucial technical point of departure between our work and [22]. While the construction of [22], reviewed briefly in Section 2.3.1 and referred to as “counting” knockoffs hereon, is valid only when the entries of $X$ are i.i.d., here we use the more general prescription of Model-X knockoffs from [8]. This effectively means that the importance statistic for a given variable involves both $\hat{\beta}_j(\lambda)$ and its knockoff counterpart, and therefore we need to study aspects of the joint distribution of these two estimates rather than just the marginal distribution of $\hat{\beta}_j(\lambda)$. For this purpose, Theorem 1 of Section 2.3 provides a significant technical extension of AMP theory that underlies our analysis but, importantly, may be of independent interest and have much broader implications. We would like to emphasize that by implementing Model-X knockoffs as originally intended, we also obviate the problem of estimating the proportion of nonnulls (i.e., the sparsity), which was a nontrivial issue to handle in [22]. Bearing these differences in mind, Table 1 illustrates where our work fits in the context of the aforementioned papers.

If we fix FDP at some level $q$, the performance of thresholded-Lasso in terms of achievable TPP may depend strongly on $\lambda$. This is demonstrated in [21], where a characterization is also
given for the value of \( \lambda \) that asymptotically maximizes TPP for a prescribed FDP level. When incorporating knockoffs, the analysis is more subtle because we operate with the difference in the estimate size between a variable and its knockoff counterpart, instead of the estimates themselves. While the dependence of the exact optimal \( \lambda \) on the unknown parameters of the problem is fairly complicated, we demonstrate that, at least in the case of i.i.d. \( X \), the optimal \( \lambda \) can be well estimated by cross-validation on the augmented design.

Figure 2 shows FDP versus TPP as predicted by the theory for Lasso and thresholded-Lasso, and for oracle/knockoffs settings. In this example, the undersampling ratio \( \delta = n/p = 0.5 \), the noise level \( \sigma = 1 \), and the signal has i.i.d. components with mass \( \epsilon = 0.1 \) at \( M = 10 \) and mass \( 1 - \epsilon = 0.9 \) at zero. The knockoffs procedures depicted use “counting” knockoffs with \( r = 0.3p \) fake columns (“knckff-count” in the legend) or Model-X knockoffs (“knckff” in the legend): for thresholded-Lasso we show both implementations; for Lasso, predictions for Model-X knockoffs are actually harder to obtain (because \( (2.3) \) is not as useful an approximation when \( W \)-statistics are considered), so we display only counting knockoffs. Comparing first the two oracles, it is clear that thresholded-Lasso has a much better ROC curve: for example, FDP is about 30% by the time Lasso detects 80% of the signals, whereas thresholded-Lasso is able to identify the true model (i.e., obtain 100% TPP with no false discoveries). Importantly, here the latter uses the optimal value for \( \lambda \), see the discussion in Section 4. Turning to the “realistic” procedures, we first observe that for thresholded-Lasso, more power is lost due to Model-X knockoffs than “counting” knockoffs. This is mainly due to the fact that in Model-X knockoffs, the number of columns in \( X \) is doubled, and the Lasso estimates consequently have larger variance. This problem is alleviated considerably when using counting knockoffs which, exploiting the i.i.d.-ness of the covariates, allow to augment \( X \) by fewer fake or control columns. Still, both versions of knockoffs for thresholded-Lasso perform substantially better than knockoffs for Lasso, and come close to the oracle thresholded-Lasso procedure. In fact, the curves for both of these procedures lie significantly below the curve for the oracle version of Lasso, and even significantly below the universal lower bound of \([15]\) on FDP (not shown in the figure). In other words, we can break through the Lasso FDP-TPP fundamental tradeoff diagram even with an FDR-calibrated thresholding-Lasso procedure, in particular with Model-X knockoffs. For example, knockoffs still attains TPP of about 90% with FDP \( \leq 5\% \). The value of \( \lambda \) used here for the knockoffs version of thresholded-Lasso is the limit of the (10-fold) cross-validation estimate (we denote it later by \( \lambda_{cv} \)).

### 1.4 Type I vs. Type S error

The classical paradigm, which is also adopted here, regards a predictor as important if the corresponding \( \beta_j \neq 0 \), and aims at controlling a Type I error rate. In practice, however, all of the underlying \( \beta_j \) are obviously different from zero to some decimal, in which case the Type I er-

|          | Lasso       | thresholded-Lasso |
|----------|-------------|-------------------|
| oracle   | Su et al (2017) | Wang et al (2017+) |
| knockoffs| Weinstein et al (2017+) | this paper |

**Table 1**
Figure 2: Theoretical predictions for Type-I error vs. power: Lasso vs. thresholded-Lasso. Oracle procedures are in blue, knockoffs (Model-X or “counting”) are in pink.

The criticism of the Type I error rate is justifiable for a procedure that has small Type I error in the stylized situation (where the nulls are actually zero) but substantially larger Type S error when the nulls are only approximately zero. In [12] this is demonstrated with respect to the standard procedure that supplements each rejection of the null (based on a two-sided p-value) with the natural decision on the sign. The procedures discussed in the current paper, however, are based on posterior probability calculations: while exact zeros are allowed in our framework a priori, our methods estimate the probability that $\beta_j = 0$ conditional on the event of selection. The resulting procedures are therefore perfectly consistent with the Bayesian options recommended in [12], which are immune to the type of “discontinuity” at zero that was mentioned above. As such, if one insists on the sign-classification framework, we explain in the concluding section how the results in this paper are reflective also of the Type S error (in a corresponding asymptotic setup), not only the Type I error, so that focusing on the latter is somewhat a choice of convenience.
2 Setup and review

2.1 Setup

Adopting the basic setting from [15], our working hypothesis entails the linear model (1.1) with $\sigma^2$ fixed and unknown, and we consider an asymptotic regime when $n, p \to \infty$ such that $n/p \to \delta > 0$. We assume that the matrix $X \in \mathbb{R}^{n \times p}$ has i.i.d. $\mathcal{N}(0, 1/n)$ entries, so that the columns are approximately normalized. The components of the coefficient vector $\beta$ are assumed to be i.i.d. copies of a mixture random variable,

$$\beta_j \sim \Pi = (1 - \epsilon)\delta_0 + \epsilon \Pi^*,$$

where $\epsilon \in (0, 1)$ is a constant, and where $\mathbb{E} \Pi^2 < \infty$. Here $\mathbb{P}(\Pi^* \neq 0) = 1$, so that $\mathbb{P}(\Pi \neq 0) = \epsilon \in (0, 1)$. With some abuse of notation, we use $\Pi, \Pi^*$ to refer to either the random variable or its distribution, but the meaning should be clear from the context. Other than having a mass at zero, $\Pi$ is completely unknown, which is to say that $\epsilon$ and $\Pi^*$ are unknown. Finally, $X, \beta$, and $\xi$ are all independent of each other.

Many selection rules first use the observed data to order the $p$ variables, that is, for some function $g$, an “importance” statistic

$$T = (T_1, \ldots, T_p)^\top = g(X, Y) \in \mathbb{R}^p$$

is computed, where larger (say) values of $T_j$ presumably indicate stronger evidence against the null hypothesis that $\beta_j = 0$. We assume that $g$ has the natural symmetry property that if $X'$ is obtained from $X$ by rearranging the columns, then $g(X', y)$ rearranges the elements of the vector $g(X, y)$ accordingly. Given a preset FDR level $q$, a final model can then be selected by taking

$$\hat{S} = \{j : T_j \geq \hat{t}\},$$

where $\hat{t} = \hat{t}(q)$ is a threshold that depends on the observed data as well as on $q$. For any choice of the importance statistic $T$ (i.e., for any choice of $g$), we define

$$\text{FDP}(t) \equiv \frac{|\{j \in H : T_j \geq t, j \in H_0\}|}{|\{j \in H : T_j \geq t\}|}, \quad \text{TPP}(t) \equiv \frac{|\{j \in H : T_j \geq t, j \notin H_0\}|}{|\{j \in H : j \notin H_0\}|}$$

(recall the convention $0/0 = 0$). In the next section we focus attention on variable selection procedures that rely on the Lasso program in computing the importance statistics.

2.2 Basic AMP predictions

We start with noting that, on defining

$$T_j = \max\{\lambda : \hat{\beta}_j(\lambda) \neq 0\},$$

we have $|\{j : T_j \geq t\}| \approx |\{j : \hat{\beta}_j(t) \neq 0\}|$, because only variables that drop out from the Lasso path—that is, for which $\hat{\beta}_j(\lambda_0) \neq 0$ but $\hat{\beta}_j(\lambda_1) = 0$ for $\lambda_1 < \lambda_0$—can contribute to the difference

\footnote{Formally, the requirement is that for any permutation $\pi$ on $(1, \ldots, p)$, $g(X_\pi, y) = [g(X, y)]_\pi$, where $X_\pi$ is defined to be the matrix with its $j$-th column equal to the $\pi(j)$-th column of $X$.}
between the quantities; see discussion in [22]. Therefore, we treat the comparison between (1.3) and (1.4) as essentially a comparison between two procedures of the form (2.1), where $T_j$ is given by (2.3) for Lasso, and by

$$T_j = |\hat{\beta}_j(\lambda)|$$

(2.4)

for thresholded-Lasso. In anticipation of Section 3 we call (2.3) the Lasso-max statistic, and we call (2.4) the Lasso-coefficient statistic.

Remarkably, under the working hypothesis, exact asymptotic predictions of FDP and TPP can be obtained for both Lasso and thresholded-Lasso. Stated informally, Theorem 1 in [3] asserts that under our working hypothesis, in the limit as $n,p \to \infty$ we can “marginally” treat

$$\left(\hat{\beta}_j, \beta_j\right) \sim \left(\eta_{\alpha \tau}(\Pi + \tau Z), \Pi\right),$$

(2.5)

and we use a dot above the “∼” symbol to indicate that this holds only in a limiting sense. Above, $\eta_\theta(x) \equiv \text{sgn}(x) \cdot (|x| - \theta)_+$ is the soft-thresholding operator (acting coordinate-wise); $Z \sim \mathcal{N}(0,1)$ and independent of $\beta$; and $\tau > 0$, $\alpha > \max\{\alpha_0, 0\}$ is the unique solution to

$$\tau^2 = \sigma^2 + \frac{1}{\delta} \mathbb{E}(\eta_{\alpha \tau}(\Pi + \tau Z) - \Pi)^2$$

$$\lambda = \left(1 - \frac{1}{\delta} \mathbb{P}(|\Pi + \tau Z| \geq \alpha \tau)\right)\alpha \tau.$$  

(2.6)

Furthermore, $\alpha_0$ is the unique root of the equation $(1 + t^2)\Phi(-t) - t\phi(t) = \delta/2$. This result underlies the analysis in [15], where it is formally shown (Lemma A.1) that

$$\frac{|\{j : \hat{\beta}_j(\lambda) \neq 0, j \in \mathcal{H}_0\}|}{p} \rightarrow 2(1 - \epsilon)\Phi(-\alpha),$$

$$\frac{|\{j : \hat{\beta}_j(\lambda) \neq 0, j \notin \mathcal{H}_0\}|}{p} \rightarrow \mathbb{P}(|\Pi + \tau Z| \geq \alpha \tau, \Pi \neq 0) = \epsilon \mathbb{P}(|\Pi^* + \tau Z| \geq \alpha \tau),$$

(2.7)

with $\alpha, \tau$ and $Z$ as described above. For a general importance statistic $T$, define

$$\text{fdp}(t) \equiv \lim \text{FDP}(t) \quad \text{tpp}(t) \equiv \lim \text{TPP}(t),$$

where the limits are in probability. We use special notation for the limiting FDP and TPP corresponding to the Lasso-max and to the Lasso-coefficient statistics we have just defined (cf. (2.3) and (2.4)). Thus, for the choice of $T_j$ in (2.3) we write $\text{fdp}^{LM}(t)$ and $\text{tpp}^{LM}(t)$, and for the choice of $T_j$ in (2.4) we write $\text{fdp}^{LC}(t; \lambda)$ and $\text{tpp}^{LC}(t; \lambda)$. In [22], (2.7) was used to approximate

$$\text{fdp}^{LM}(t) \approx \frac{2(1 - \epsilon)\Phi(-\alpha)}{2(1 - \epsilon)\Phi(-\alpha) + \epsilon \mathbb{P}(|\Pi^* + \tau Z| \geq \alpha \tau)}$$

$$\text{tpp}^{LM}(t) \approx \mathbb{P}(|\Pi^* + \tau Z| \geq \alpha \tau),$$

(2.8)

where $(\alpha, \tau)$ are the solution to (2.6) on replacing $\lambda$ by $t$.

In a more recent work, [21] observed that the implications of [3] can, with the necessary adaptations, be used to analyze TPP and FDP also for thresholded-Lasso. Thus, Lemma 2.2 in [21]
asserts that
\[
\frac{|\{j : \hat{\beta}_j(\lambda) \geq t, j \in \mathcal{H}_0\}|}{p} \xrightarrow{p} 2(1 - \epsilon)\Phi(-\alpha - t/\tau)
\]
\[
\frac{|\{j : \hat{\beta}_j(\lambda) \geq t, j \notin \mathcal{H}_0\}|}{p} \xrightarrow{p} \epsilon P(\|\Pi^\ast + \tau Z\| \geq t + \alpha t).
\]  
(2.9)

It then follows that
\[\text{fdp}^{LC}(t; \lambda) = \frac{2(1 - \epsilon)\Phi(-\alpha - t/\tau)}{2(1 - \epsilon)\Phi(-\alpha - t/\tau) + \epsilon P(\|\Pi^\ast/\tau + Z\| \geq \alpha + t/\tau)},\]
\[\text{tpp}^{LC}(t; \lambda) = P(\|\Pi^\ast/\tau + Z\| \geq \alpha + t/\tau),\]
(2.10)

where \((\alpha, \tau)\) are determined by \(\lambda\) through (2.6). Hence, the asymptotic TPP and FDP in (2.10) depend on the value of \(\lambda\) at which the Lasso estimates are computed. Theorem 3.2 in [21] further identifies the asymptotically optimal value of \(\lambda\), proving that for any \(\lambda > 0\),
\[\text{tpp}^{LC}(t; \lambda^\ast) \leq \text{tpp}^{LC}(t; \lambda) \implies \text{fdp}^{LC}(t; \lambda^\ast) \leq \text{fdp}^{LC}(t; \lambda),\]
where
\[\lambda^\ast = \arg\min_{\lambda} \frac{1}{p} \|\hat{\beta}(\lambda) - \beta\|_2.\]  
(2.11)

By inspection, we see that an equivalent characterization of \(\lambda^\ast\) is the value of \(\lambda\) corresponding to the minimum \(\tau\) in (2.6). This characterization is useful for computing \(\lambda^\ast\) as a function of \(\epsilon, \Pi^\ast, \sigma^2\).

Comparing the curves \(t \mapsto (\text{tpp}(t), \text{fdp}(t))\) corresponding to (2.8) and (2.10), [21] concluded that with an appropriate choice of \(\lambda\), thresholded-Lasso can improve significantly over Lasso, in the sense that a target TPP level can be achieved with much smaller FDP, and as illustrated by the dotted curves in Figure 2.

2.3 Knockoffs for FDR control

The choice of an adequate feature importance statistic is crucial for producing a good ordering of the \(\beta_j\)'s, from the most likely to be nonnull to the least likely to be nonnull. A separate question is how to set the threshold \(\hat{t}\) in (2.1) so that the FDR is controlled at a prespecified level. Inspired by [1], [8] proposed a general method for the random-X setting, Model-X knockoffs, that utilizes artificial null variables for finite-sample control of the FDR. Assuming that the distribution of \(X_i\) is known, the basic idea is to introduce, for each of the \(p\) original variables, a fake control so that complete exchangeability holds under the null. In other words, if \(\beta_j = 0\), then the importance statistic for the \(j\)-th variable is indistinguishable from that corresponding to its fake copy. This property can then be exploited by keeping track of the number of fake variables selected as an estimate for the number of false positives.

Under our working assumptions, the random variables \(X_{i1}, \ldots, X_{ip}\) are i.i.d., in which case the construction of Model-X knockoffs is trivial. Thus, let now \(\tilde{X} \in \mathbb{R}^{n \times p}\) be a matrix with i.i.d. \(\mathcal{N}(0, 1/n)\) entries drawn completely independently of \(X, \xi\) and \(\beta\), so that it holds in particular that \(Y\) and \(\tilde{X}\) are independent conditionally on \(X\). We refer to \([X, \tilde{X}] \in \mathbb{R}^{n \times 2p}\) as the augmented \(X\)-matrix.
Ranking of the original $p$ features is based on contrasting the importance statistic for variable $j$ with that for its knockoff counterpart where, crucially, all importance statistics are computed on the augmented matrix. Specifically, the Lasso coefficient-difference (LCD) statistic [8] is

$$W_j = |\hat{\beta}_j(\lambda)| - |\hat{\beta}_{p+j}(\lambda)|,$$  \hspace{1cm} (2.12)

where

$$\hat{\beta}(\lambda) = \arg\min_{b \in \mathbb{R}^p} \frac{1}{2} \|Y - [X, \tilde{X}]b\|_2^2 + \lambda \|b\|_1$$  \hspace{1cm} (2.13)

is the Lasso solution for the augmented $X$ matrix.

Because $\tilde{X}$ is a valid matrix of Model-X knockoffs, we have from Lemma 3.3. in [8] that the signs of the $W_j, j \in H_0,$ are i.i.d. coin flips (in fact, when $X_{ij}, j = 1, ..., p,$ are i.i.d., as considered here, this is easy to see directly from symmetry). In the knockoffs framework, variables are selected when their $W_j$ is large, that is,

$$\hat{S} = \{j : W_j \geq \hat{t}\},$$  \hspace{1cm} (2.14)

where $\hat{t}$ is a data-dependent threshold. The idea is to rely on the “flip-sign” property of the $W_j$ to choose $\hat{t}$. Concretely, applying the knockoff filter by putting

$$\hat{t} = \min \left\{ t > 0 : \hat{\text{FDP}}(t) \leq q \right\}, \hspace{1cm} \hat{\text{FDP}}(t) \equiv \frac{1 + \# \{j : W_j \leq -t\}}{\# \{j : W_j \geq t\}},$$  \hspace{1cm} (2.15)

ensures that the selection rule given by (2.14) controls the FDR at level $q$ by Theorem 3.4 in [8]. The above is summarized in the following

**Definition 2.1.** The level-$q$ LCD-knockoffs procedure is the multiple testing procedure given by (2.14) with the choice of $W_j$ in (2.12), and with $\hat{t}$ given by (2.15).

Consistent with the notation in Section 2, we write $\hat{\text{fdp}}^{LCD}(t), \hat{\text{tpp}}^{LCD}(t),$ respectively, for $\text{fdp}(t)$ and $\text{tpp}(t)$ associated with the statistic (2.12). Finally, let

$$\hat{\text{fdp}}^{LCD}(t) \equiv \lim \hat{\text{FDP}}(t)$$

be the limit of the (knockoffs) estimate of FDP given in (2.15).

Before proceeding to the main section, we recall an alternative implementation of knockoffs for the special case of i.i.d. matrices.

**2.3.1 “Counting” knockoffs for i.i.d. matrices**

In the special case where $X_{i1}, ..., X_{ip}$ are i.i.d., there is in fact a simpler approach to implementing a knockoff procedure, as proposed in [22]. Instead of pairing each original covariate with a designated knockoff copy ($X_j$ with $\tilde{X}_j$), we can leverage the information that the covariates are i.i.d., and therefore exchangeable, to create a single pool of knockoff variables $\tilde{X}_1, ..., \tilde{X}_r$ that act as a “control group” simultaneously for each $X_1, ..., X_p$.

To be concrete, for some integer $r > 0,$ suppose we make the matrix $\tilde{X}$ of dimension $n \times r$ instead of $n \times p,$ still with i.i.d. $\mathcal{N}(0, 1/n)$ entries as before. Then by the symmetry in the problem,
the distribution of the fitted coefficient vector \( \hat{\beta}_1, \ldots, \hat{\beta}_{p+r} \) (conditional on \( \beta \)) is unchanged under any reordering of the indices in the “extended” null set,

\[ \mathcal{H}_0 \cup \mathcal{K}_0, \]

where \( \mathcal{K}_0 = \{p+1, \ldots, p+r\} \). This is a stronger notion of exchangeability (all null covariates are exchangeable with all knockoff variables), as compared to the pairwise exchangeability property of the general Model-X framework (where each null \( X_j \) is only exchangeable with its own knockoff copy \( \tilde{X}_j \)). Exploiting this stronger form of exchangeability, [22] prove FDR control—for example, we could take the procedure that rejects \( H_{0j} \) whenever \( \hat{\beta}_j \geq \hat{t} \) for

\[
\hat{t} = \inf \left\{ t \in \mathbb{R} : \frac{1}{p+1} \sum_{j \in \mathcal{K}_0} 1\{\hat{\beta}_j > t\} \leq q \right\},
\]

and use AMP machinery to derive the appropriate formulas for the power. In particular, power is gained from the fact that, if we choose \( r \) to be smaller than \( p \) (e.g., \( r = c \cdot p \) for some \( 0 < c < 1 \)), the variable selection accuracy of the Lasso is better since we have \( n \) observations and \( p + r = p(1 + c) \) many covariates, rather than \( n \) observations and \( 2p \) covariates as with Model-X knockoffs.

However, the “counting knockoffs” strategy is extremely specific to the i.i.d. design setting: if the \( X_j \)'s are not themselves i.i.d. (or exchangeable), then we cannot hope to construct a single control group that can be shared by a heterogeneous set of covariates. The Model-X construction, with knockoff \( \tilde{X}_j \) designed to pair with \( X_j \), is therefore substantially more interesting to study in terms of understanding the performance of this methodology in non-i.i.d. settings (even though we study Model-X with an i.i.d. design due to the assumptions of the AMP tools underlying our power calculations). On the other hand, the paired construction of Model-X knockoffs necessitates new AMP theory to be able to quantify its performance.

### 3 AMP predictions for knockoffs

The results presented thus far are not novel. In this section we study the level-\( q \) LCD-knockoffs procedure theoretically, and present new results. For the knockoffs procedure to control the FDR, the i.i.d. Gaussian assumption on the \( p \) coordinates of \( X_i \) is by no means necessary, and there is indeed no such assumption in [8]. In this paper, on the other hand, the aim is to evaluate how much power is lost due to knockoffs by comparing, qualitatively and quantitatively, the asymptotically attainable power for the Lasso-coefficient statistic with and without knockoffs. More formally, the goal is ultimately to compare the curves

\[
q \mapsto \text{tpp}^{LC}(t^{\infty}(q)), \quad q \mapsto \text{tpp}^{LCD}(\hat{t}^{\infty}(q)),
\]

where the quantities \( t^{\infty}(q) \) and \( \hat{t}^{\infty}(q) \) are defined, respectively, as the values \( t^{\infty} \) and \( \hat{t}^{\infty} \) for which

\[
\text{fdp}^{LC}(t^{\infty}) = q, \quad \text{fdp}^{LCD}(\hat{t}^{\infty}) = q.
\]

Of course, how the two curves in (3.1) compare on power at every given \( q \), depends on the underlying model, including the dependence structure among the coordinates of \( X_i \). Similarly to [15] [21], we

---

2 We note that, while [22] focus on a different statistic, all of their results concerning FDR control apply equally well to what we call the Lasso-coefficient statistic in the following section.
work in the setting of i.i.d. Gaussian covariates only because we currently do not have the machinery to conduct an asymptotic analysis beyond this setting.

As already mentioned in the Introduction, while the results in [15, 21, 22] rely fundamentally on the theory in [4], a highly nontrivial extension is required for the analysis in the current paper. The main technical challenge is to validate that the theory from [4] carries over to the knockoff setup involving \( W \)-statistics. In essence, we are looking to establish that, for our purposes, we can asymptotically treat

\[
\left( \hat{\beta}_j, \beta_j, \tilde{\beta}_{p+j} \right) \sim \left( \eta_{\alpha', \tau'}(\Pi + \tau'Z), \Pi, \eta_{\alpha', \tau'}(\tau'Z') \right),
\]

where \( Z \) and \( Z' \) are independent \( \mathcal{N}(0, 1) \) random variables that are furthermore independent of \( \beta_j \), and where \((\alpha', \tau')\) are independent random variables that are furthermore independent of \( \beta_j \), and \( (\alpha', \tau') \) are given by the unique solution for \((\alpha, \tau)\) in

\[
\begin{align*}
\tau^2 &= \sigma^2 + \frac{1}{\delta} \mathbb{E} \left[ \eta_{\alpha \tau}(\Pi + \tau Z) - \Pi \right]^2 + \frac{1}{\delta} \mathbb{E} \eta_{\alpha \tau}(\tau Z)^2 \\
\lambda &= \left[ 1 - \frac{1}{\delta} \mathbb{P}(|\Pi + \tau Z| > \alpha \tau) - \frac{1}{\delta} \mathbb{P}(|\tau Z| > \alpha \tau) \right] \alpha \tau.
\end{align*}
\]

Thus, as compared to (2.5), we now need to study the triples \( (\hat{\beta}_j, \beta_j, \tilde{\beta}_{p+j}) \) rather than the pairs \( (\hat{\beta}_j, \beta_j) \). The following theorem formalizes the notion in which (3.3) holds, and constitutes our main theoretical result.

**Theorem 1.** Let \( f \) be any bounded continuous function defined on \( \mathbb{R}^3 \). Then, we have

\[
\frac{1}{p} \sum_{i=1}^{p} f(\beta_i, \beta_j, \tilde{\beta}_{p+i}) \to \mathbb{E} f(\eta_{\alpha', \tau'}(\Pi + \tau'Z), \Pi, \eta_{\alpha', \tau'}(\tau'Z'))
\]

in probability. Here and throughout, \((\alpha', \tau')\) are the unique solution to (3.4), and \( Z \) and \( Z' \) are two independent standard normal random variables, which are further independent of \( \Pi \). Moreover, the convergence in probability is uniform over \( \lambda \) in any compact set of \((0, \infty)\).

This result is closely related to Corollary 1 in [3] which in a sense is a “marginal” version of Theorem 1. In the Model-X knockoffs context, [3] implies the convergence of a sum over all pairs \( i, j \) such that \( 1 \leq i, j \leq 2p \), as opposed to “diagonal” pairs \( i, p + i \) for \( 1 \leq i \leq p \) in Theorem 1 above. Corollary 1 in [3] then follows by making use of its conditional (hence stronger) counterpart, Theorem 1. More generally, just as Corollary 1 in [3] applies to a tuple of any number of indices, Theorem 1 can be readily extended to multiple knockoffs (where several knockoff copies are generated for each original variable). This extension would allow for a theoretical comparison similar to that presented in the current paper except with multiple knockoffs, and we leave this interesting direction for future research.

Theorem 1 allows us to calculate the limits of TPP\((t)\) and FDP\((t)\) for the LCD statistic at any fixed threshold value \( t \).

**Corollary 3.1.** Fix \( \lambda > 0 \). Then for any \( t > 0 \),

\[
\begin{align*}
\text{fdp}^{\text{LCD}}(t) &= \frac{(1 - \epsilon) \mathbb{P}(|\tau' \eta_{\alpha'}(Z)| - |\tau' \eta_{\alpha'}(Z')| \geq t)}{\mathbb{P}(|\eta_{\alpha', \tau'}(\Pi + \tau'Z)| - |\tau' \eta_{\alpha'}(Z')| \geq t)} \\
\text{tpp}^{\text{LCD}}(t) &= \mathbb{P}(|\eta_{\alpha', \tau'}(\Pi + \tau'Z)| - |\tau' \eta_{\alpha'}(Z')| \geq t|\Pi \neq 0).
\end{align*}
\]
Moreover, Theorem 1 allows us to calculate the limit of the knockoffs estimate of $\text{FDP}(t)$ for any fixed $t$:

**Corollary 3.2.** Fix $\lambda > 0$. Then for any $t > 0$, the limit of $\hat{\text{FDP}}(t)$ is

$$
\hat{\text{fdp}}^{\text{LCD}}(t) = \frac{\mathbb{P}(|\eta_{\alpha'}(\Pi + \tau'Z)| - |\tau'\eta_{\alpha'}(Z')| \leq -t)}{\mathbb{P}(|\eta_{\alpha'}(\Pi + \tau'Z)| - |\tau'\eta_{\alpha'}(Z')| \geq t)}.
$$

(3.6)

From Corollaries 3.2 and 3.1 we can calculate $\text{tpp}^{\text{LCD}}(\hat{t}^\infty(q))$, the asymptotic TPP achievable by the level-$q$ LCD-knockoffs procedure: for a given $q$, first compute $\hat{t}^\infty$ using (3.6), and then plug it into the second equation in (3.5) to find $\text{tpp}^{\text{LCD}}(\hat{t}^\infty)$. It is easy to verify the relationship

$$
\hat{\text{fdp}}^{\text{LCD}}(t) = \text{fdp}^{\text{LCD}}(t) + \frac{\epsilon \mathbb{P}(|\eta_{\alpha'}(\Pi + \tau'Z)| - |\tau'\eta_{\alpha'}(Z')| \leq -t|\Pi \neq 0)}{\mathbb{P}(|\eta_{\alpha'}(\Pi + \tau'Z)| - |\tau'\eta_{\alpha'}(Z')| \geq t)},
$$

(3.7)

so that $\hat{\text{fdp}}^{\text{LCD}}(t)$ overestimates the actual asymptotic FDP, $\text{fdp}^{\text{LCD}}(t)$. However, the difference between the two is typically very small: because the random variable $|\eta_{\alpha'}(\Pi + \tau'Z)| - |\tau'\eta_{\alpha'}(Z')|$ is designed to tend to large values given that $\Pi \neq 0$, the second term on the right hand side of (3.7) is typically much smaller than $\epsilon$, for example it converges to zero when the magnitude of nonzero elements of $\beta$ increases. In other words, the fact that it is the observable random variable $\hat{\text{FDP}}(t)$—not FDP($t$)—that is used in (2.15), does not make LCD-knockoffs overly conservative. We note that the conservativeness was a nuisance in the (alternative) “counting” knockoffs implementation in [22], where an estimate of $\epsilon$ was incorporated to mitigate the effect. Here, conveniently, the use of $W$-statistics obviates the need to estimate $\epsilon$.

Figure 3 shows the “knockoffs” power $\text{tpp}^{\text{LCD}}(\hat{t}^\infty(q))$ against the “oracle” power $\text{tpp}^{\text{LC}}(\hat{t}^\infty(q))$, when the nominal FDR value $q$ varies. The tuning parameter $\lambda$ is selected separately for each procedure: for the oracle, this is the optimal $\lambda$ obtained by minimizing the value of $\tau$; for knockoffs, we use the limit $\lambda_{cv}$ of the (10-fold) cross-validation estimate, see Section 4. We can see that for $\delta \geq 1$, the powers obtained by knockoffs and the oracle are very similar for any $q$. The loss of power is more pronounced when $\delta$ decreases. However, for all considered values of $\delta$ the power of knockoffs is a convex function of the oracle power, which shows that the relative difference decreases with power of the oracle (i.e. when $q$ or the magnitude of nonzero elements of $\beta$ increase). The dotted curves in Figure 3 are the analogs of the solid black curves, when the “counting” knockoffs are implemented instead of Model-X knockoffs (we took $r = 0.3p$ here as in Figure 2). We can see that the loss in power, as compared to the oracle, is even smaller in that case.

Figure 4 complements Figure 3 by showing FDP-TPP tradeoff paths from a simulation, in addition to the theoretical predictions. For each version of thresholded-Lasso (knockoffs/oracle) we plotted 15 realizations of the tradeoff curves in an example with $n = p = 1$, $\sigma = 1$ and $\Pi$ has mass 0.9 at zero and mass 0.1 at $M = 4$. To avoid overloading the figure, we plot only the paths for Model-X knockoffs and not for counting knockoffs. We can see a good agreement between the empirical results and the theory.

We conclude this section with Theorem 2 below that formalizes the notion that the LCD-knockoffs procedure breaks through the FDP-TPP diagram of [15]. More specifically, we show that for any nominal FDR level $q > 0$ that is not too close to 1, the LCD-knockoffs procedure has asymptotic power arbitrarily close to one, as long as the signal sparsity is below the Donoho-Tanner transition curve [10] (adjusted to the size of the augmented matrix) and provided that the signal is strong enough.
Figure 3: The parametric curve \( q \mapsto (\text{tpp}^{L_C}(t^{\infty}(q)), \text{tpp}^{L_{CD}}(\hat{t}^{\infty}(q))) \). Dotted curve is the counterpart for the “counting” knockoffs of Section 2.3.1. Each panel corresponds to a different value of \( \delta \): from top left and clockwise, \( \delta = 0.5, 1, 1.5, 2 \). In all panels, \( \sigma = 1 \) and \( \Pi \) has mass 0.9 at zero and mass 0.1 at \( M = 4 \). Pink segments indicate \( q = 0.01 \) (closest to origin), 0.05 and 0.1 (farthest from origin).
**Figure 4:** FDP-TPP tradeoff curves for thresholded-Lasso in a simulated example. Light, thin lines represent (random) realizations from 15 simulated runs. Dark, thick lines are theoretical predictions.

**Definition 3.3.** A sequence of random variables $\Pi_m$ is said to be $\epsilon$-sparse and growing, if $\mathbb{P}(\Pi_m \neq 0) = \epsilon$ for all $m$, and
\[
\mathbb{P}(|\Pi_m| > M | \Pi_m \neq 0) \to 1
\]
as $m \to \infty$ for every $M > 0$.

**Theorem 2.** Let $W_j(\lambda) = |\hat{\beta}_j(\lambda)| - |\hat{\beta}_{p+j}(\lambda)|$. Fix $q > 0$ and denote by $\text{TPP}(\lambda, \Pi, q)$ the true positive proportion of the level-$q$ LCD-knockoffs procedure using parameter $\lambda$. Then for any sequence $\{\Pi_m\}$ that is $\epsilon$-sparse and growing, it holds that for any fixed $0 < \lambda_1 < \lambda_2$ and any $\nu > 0$, there exist $m'$ and $n'(m)$ such that
\[
\mathbb{P}
\left(\inf_{\lambda_1 \leq \lambda \leq \lambda_2} \text{TPP}(\lambda, \Pi_m, q) > 1 - \nu\right) \geq 1 - \nu
\]
if $m \geq m'$ and $n \geq n'(m)$.

**4 Tuning by cross-validation**

The level-$q$ LCD-knockoffs procedure requires specification of $\lambda$, the tuning parameter in (2.13), and the resulting power may indeed vary considerably with the choice of $\lambda$. For the Lasso-coefficient (“oracle”) procedure, operating on the original $n \times p$ matrix, [21] characterized the asymptotically optimal value of $\lambda$. Specifically, let $\text{tpp}^{LC}(\lambda) \equiv \text{tpp}^{LC}(t(\lambda); \lambda)$, where $t(\lambda)$ is the smallest positive value such that $\text{fdp}^{LC}(t(\lambda); \lambda) \leq q$. Then Theorem 3.2 in [21] asserts that, for any $q$,
\[
\lambda \text{ maximizes } \text{tpp}^{LC}(\lambda) \iff \lambda \text{ minimizes } \lim_{p} \frac{1}{p} \|\hat{\beta} - \beta\|_2^2.
\]
In words, asymptotically, the value of $\lambda$ minimizing the estimation mean squared error (MSE) is also the optimal $\lambda$ for the testing problem. \cite{21} then observe that minimizing the limiting estimation error, $\mathbb{E}[(\eta_{\tau}(\Pi + \tau Z) - \Pi)^2]$, is in turn equivalent to minimizing $\tau$ in (2.6) over $\lambda$. As the minimizer of $\tau$ depends on $\Pi$ and $\sigma$, \cite{21} propose to estimate $\lambda$ in practice by minimizing a consistent estimate of $\tau$.

If the only difference between knockoffs and the oracle were the fact that the augmented $X$-matrix is used instead of the original $X$-matrix, we would be able to conclude immediately that the optimal tuning parameter for LCD-knockoffs is the value of $\lambda$ minimizing $\tau$ in (3.4) instead of (2.6). This is, however, not the only difference, first because knockoffs use $W$-statistics instead of $\hat{\beta}$, and secondly because knockoffs utilize an estimate of FDP instead of the actual FDP in setting the threshold. Admittedly, the exact value of $\lambda$ that is optimal for knockoffs no longer has such a simple characterization, but we can still advocate the $\lambda$ minimizing $\tau$ in (3.4) as a good approximation, and this is our target. Figure 5 demonstrates that this approximation is indeed a good one.

The value of $\lambda$ minimizing $\tau$ in (3.4) again depends on the unknown $\Pi$ and $\sigma$. To estimate it, instead of relying on a consistent estimator of $\tau$ as in \cite{21}, we propose to use cross-validation on the augmented design. This takes advantage of the fact that when the covariates are i.i.d., minimizing the estimation error is equivalent to minimizing the prediction error. Hence, from now on we write $\lambda_{cv}$ for the $K$-fold cross-validation estimate of $\lambda$ operating on the augmented $X$-matrix. We can again predict the exact limit of $\lambda_{cv}$ as follows.

**Lemma 4.1.** For fixed $\Pi$, let $\tau(\lambda; \delta)$ be the solution in $\tau$ to (3.4) as a function of $\lambda$ and $\delta$. Then $\lambda_{cv}$ converges in probability to a constant, call it $\lambda_{cv}$. Furthermore,

$$\lambda_{cv} = \arg\min_{\lambda} \tau(\lambda; (K - 1)\delta/K),$$

(4.1)

where we note that minimizing $\tau$ in (3.4) for $\delta, \epsilon, \Pi^*$, is equivalent to minimizing $\tau$ in (2.6) for $\delta/2, \epsilon/2, \Pi^*$.

How to obtain $\lambda_{cv}$ is not immediate from Lemma 4.1 for any value of $\lambda$. $\tau$ is itself given implicitly as the solution to an equation system in two variables, which then needs to be minimized over $\lambda$. We can nevertheless define a simple procedure for solving this minimization problem, described in Appendix B and ultimately yielding the system of equations

$$\tau_{cv}^2 = \sigma^2 + \frac{K}{(K - 1)\delta} \mathbb{E}[\eta_{\alpha_{cv}^*}(\Pi + \tau_{cv}Z - \Pi)]^2 + \frac{K}{(K - 1)\delta} \mathbb{E}[\eta_{\alpha_{cv}^*}(\tau_{cv}Z)]^2,$$

$$2\varphi(\alpha_{cv}) - 2\alpha_{cv}\Phi(-\alpha_{cv}) = \mathbb{E}[Z + \alpha_{cv}; \Pi + \tau_{cv}Z < -\tau_{cv}\alpha_{cv}] - \mathbb{E}[Z - \alpha_{cv}; \Pi + \tau_{cv}Z > \tau_{cv}\alpha_{cv}].$$

(4.2)

We call (4.2) the CV-AMP equations. To obtain $\lambda_{cv}$, we solve the CV-AMP equations, and then use the second equation of (3.4) with $(K - 1)\delta/K$ substituted for $\delta$ and with $\tau_{cv}$ substituted for $\tau$.

Figure 5 shows power against $\lambda$ for the LCD-knockoffs procedure applied at level $q = 0.1$. For reference, horizontal lines indicate theoretical power for the knockoffs procedure utilizing the Lasso-max statistic (2.3) (computed on the augmented matrix). The latter is obtained from \cite{22} and uses “counting” knockoffs with the true underlying value of $\epsilon$. For LCD, the theoretical predictions are consistent with the simulation results (marker overlays), and demonstrate how drastically power can vary with the choice of the tuning parameter. In particular, bad choices of $\lambda$ can lead to smaller power than even the knockoffs version of Lasso (1.3). Vertical solid lines indicate the value of $\lambda_{cv}$,
Figure 5: Power versus $\lambda$ for the level-$q$ LCD-knockoffs procedure, $q = 0.1$. Light blue curves are theoretical predictions for TPP, marker overlays are averages over $N = 100$ simulation runs with $\sigma = 1$, $n = p = 5000$, and $\Pi$ has mass $1 - \epsilon$ at zero and mass $\epsilon$ at $M = 5$ ($\epsilon$ varies between panels). Horizontal red lines indicate predicted TPP for the (“counting”) knockoffs procedure using the Lasso-max statistic (2.3). The solid vertical line is the theoretical limit $\lambda_{cv}$, and the broken vertical line is the simulation average, for the cross-validation estimate of $\lambda$ with $K = 10$ folds.

Figure 6: Sampling variability in estimating $\lambda$: CV versus the method of [21]. Boxplots are based on 1000 simulation runs.

and they indeed seem close to optimal, i.e., close to the value that maximizes power. The broken vertical lines represent the simulation average for the 10-fold cross-validation $\lambda$.

The boxplots in Figure 6 show sampling variability in 1000 simulation runs for the cross-validation estimate of $\lambda$ and for the estimate of [21]. In all panels we used $n = 1000$, $p = 1500$, and $\Pi$ has mass $1 - \epsilon = 0.9$ at zero and mass $\epsilon = 0.1$ at $M = 5$. The red horizontal line indicates $\lambda_{cv}$ for $\delta = n/p = 2/3$. Sampling variability for cross-validation appears smaller. Another (unrelated) advantage of cross-validation is that we have an explicit characterization of $\lambda_{cv}$ through the CV-AMP equations, whereas the analog for the method of [21] is given implicitly as a minimizer of a certain estimate.
5 Extension to Type S errors

As implied in the introduction, the calculations throughout can be converted to represent the power for directional decisions instead of point testing under a suitable asymptotic setup. Here we describe briefly analogous implications for Type S error in an adequate asymptotic setup. For Lasso and for thresholded-Lasso consider the corresponding procedures that supplement each selection $j \in \hat{S}$ with the natural estimate $\text{sgn}(\hat{\beta}_j)$ for the sign of $\beta_j$. In general, define the false sign proportion (FSP, with reference to [14]) to be the ratio of the number of directional errors to $|\hat{S}|$, and define the true sign proportion (TSP) to be the ratio of correct sign classifications to the number of nonzero $\beta_j$. Now suppose, for example, that

$$
\beta_j \sim \Pi = \begin{cases}
\Pi^*, & \text{w.p. } \epsilon \\
\mathcal{N}(0, \gamma), & \text{w.p. } (1 - \epsilon)(1 - \epsilon') \\
0, & \text{w.p. } (1 - \epsilon)\epsilon'
\end{cases}
$$

(5.1)

Hence, the mass $1 - \epsilon$ is now divided between zero and a continuous distribution symmetric about zero, here taken to be Gaussian. For simplicity, assume also that $\mathbb{P}(\Pi^* > 0) = 1$, otherwise we would distinguish between the positive part and negative part of $\Pi^*$ and proceed as follows. Then, using results from [2], it can be shown that in the augmented setup

$$
\lim_{\epsilon' \to 0} \lim_{\gamma \to 0} \lim_{n \to \infty} \text{FSP}(t) = \frac{1}{2} \lim_{n \to \infty} \text{FDP}(t),
$$

and that the same holds when replacing FSP($t$) with $\text{FSP}(t)$, the knockoffs estimate of FSP. Note in particular that the limit of FSP($t$) is not larger than the limit for FDP($t$) (in fact, it is smaller by a factor of two because, for every single parameter, there is only one direction for error); this confirms the qualitative assertions from Subsection 1.4. Similarly, the limiting power for sign detection would be

$$
\lim_{\epsilon' \to 0} \lim_{\gamma \to 0} \lim_{n \to \infty} \text{TSP}(t) = \epsilon \mathbb{P}(|\eta_{\alpha'}(\Pi^* + \tau'Z)| - |\tau'\eta_{\alpha'}(Z')| \geq t) - \\
(1 - \epsilon)\epsilon' \mathbb{P}(\eta_{\alpha'}(\Pi^* + \tau'Z) < 0) + \frac{1}{2}(1 - \epsilon) \lim_{n \to \infty} \text{TPP}(t).
$$

The second term on the right hand side can be regarded as the Type III error, the probability that a “truly” nonzero parameter is coincidently selected with a wrong sign. The above formulas can be used to modify the tradeoff diagrams for the knockoffs version of thresholded-Lasso in, e.g., Figure 2.

Acknowledgement

A. W. is supported by ISF via grant 039-9325. W. S. is partially supported by NSF via grant CCF-1934876, and by the Wharton Dean’s Research Fund. M. B. is supported by the Polish National Center of Science via grant 2016/23/B/ST1/00454. R. F. B. is supported by NSF via grant DMS-1654076, and by the Office of Naval Research via grant N00014-20-1-2337. E. C. is partially supported by NSF via grants DMS 1712800 and DMS 1934578.
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A Proofs

Our aim in this appendix is to prove Theorems 1 and 2. The proofs rely heavily on some extensions of AMP theory and approximation results for continuous functions, which we first present in Section A.1 and the beginning of Section A.2 respectively.

A.1 Local AMP lemmas

Following the setting of AMP theory as specified earlier in Section 2, we present some extensions of AMP theory for the Lasso method. We call these results local AMP lemmas in view of the fact that these results apply to some subset of the coordinates of the coefficients, as opposed to applying all coordinates symmetrically by the existing AMP results.

Hereafter in this appendix, we use \( \xrightarrow{p, \alpha} \) to denote convergence in probability for simplicity. Recall that \( \alpha' \), \( \tau' \) are the unique solutions to the set of equations (3.4).

Lemma A.1. Let \( g : \mathbb{R}^2 \rightarrow \mathbb{R} \) and \( h : \mathbb{R} \rightarrow \mathbb{R} \) be two bounded continuous functions. We have

\[
\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \xrightarrow{p, \alpha} E \left[ g(\eta_{\alpha' \tau'}(\Pi + \tau' Z), \Pi) \right] \cdot E \left[ h(\eta_{\alpha' \tau'}(\tau' Z)) \right].
\]
Lemma A.1 is the main contribution of this subsection. Its proof depends on the following three lemmas and we defer the proofs of these preparatory lemmas later in this subsection.

**Lemma A.2.** Let $f : \mathbb{R} \to \mathbb{R}$ be any bounded continuous function. We have

$$\frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) \xrightarrow{p} \mathbb{E} f(\eta_{\alpha'\tau'}(\tau' Z)).$$

**Lemma A.3.** Let $f : \mathbb{R}^2 \to \mathbb{R}$ be any bounded bivariate continuous function. We have

$$\frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_i, \beta_i) \xrightarrow{p} \mathbb{E} f(\eta_{\alpha'\tau'}(\Pi + \tau' Z), \Pi).$$

**Lemma A.4.** For any numbers $A_1, \ldots, A_p$ and $B_1, \ldots, B_p$, denote by $\bar{A}$ and $\bar{B}$ their sample means, respectively. Let $\pi$ be drawn from all permutations of $1, \ldots, p$ uniformly at random. Then, we have

$$\text{Var}(A_1 B_{\pi(1)} + \cdots + A_p B_{\pi(p)}) = \frac{\left[ \sum_{i=1}^{p} (B_i - \bar{B})^2 \right] \left[ \sum_{i=1}^{p} (A_i - \bar{A})^2 \right]}{p - 1}.$$

**Proof of Lemma A.1.** By Lemma A.2 we have

$$\frac{1}{p} \sum_{i=1}^{p} h(\hat{\beta}_{p+i}) \xrightarrow{p} \mathbb{E} \left[ h(\eta_{\alpha'\tau'}(\tau' Z)) \right],$$

and Lemma A.3 gives

$$\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) \xrightarrow{p} \mathbb{E} \left[ g(\eta_{\alpha'\tau'}(\Pi + \tau' Z), \Pi) \right].$$

Now, let us consider the distribution of

$$\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \quad (A.1)$$

classical on $g(\hat{\beta}_1, \beta_1), \ldots, g(\hat{\beta}_p, \beta_p)$ and the empirical distribution of $\{h(\hat{\beta}_{p+i})\}_{i=1}^{p}$. This $\sigma$-algebra is denoted as $\mathcal{F}$. Note that knowing the empirical distribution of $\{h(\hat{\beta}_{p+i})\}_{i=1}^{p}$ is the same as knowing all values of $h(\hat{\beta}_{p+i})$ but the indices. For this, we need Lemma A.4 and recognize that the conditional distribution of (A.1) is the same as

$$\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+\pi(i)}),$$

where $(\pi(1), \ldots, \pi(p))$ is a permutation of $1, \ldots, p$ drawn uniformly at random. Then, first we know

$$\mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+\pi(i)}) \bigg| \mathcal{F} \right] = \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) \right] \left[ \frac{1}{p} \sum_{i=1}^{p} h(\hat{\beta}_{p+i}) \right],$$

which converges to the constant

$$\mathbb{E} \left[ g(\eta_{\alpha'\tau'}(\Pi + \tau' Z), \Pi) \right] \mathbb{E} \left[ h(\eta_{\alpha'\tau'}(\tau' Z)) \right].$$
Recognizing the boundedness of $\sum gh/p$, which results from the boundedness of the terms of this sum, a consequence of the above implies

$$\text{Var}\left\{ \mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \mid \mathcal{F} \right] \right\} \to 0. \tag{A.2}$$

Moreover, due to the boundedness of $\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i})$, it must hold that

$$\mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right] = \mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right] \xrightarrow{p} \mathbb{E} \left[ g(\eta_{\alpha' \tau'}(\Pi + \tau' Z), \Pi) \right] \mathbb{E} \left[ h(\eta_{\alpha' \tau'}(\tau' Z)) \right]. \tag{A.3}$$

Now, we consider the variance and write $\|f\|_{\infty}$ for the supremum of a function $f$. To begin, we invoke Lemma A.4, from which we get

$$\text{Var} \left\{ \mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right] \right\} = \sum_{i=1}^{p} \mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right]$$

$$= \sum_{i=1}^{p} \mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right] \leq \frac{16p^2 \|g\|_{2\infty}^2 \|h\|_{2\infty}^2}{p^2 (p-1)} \leq 0 \as p \to \infty.$$ 

as $p \to \infty$. Therefore, its boundedness gives

$$\mathbb{E} \left\{ \text{Var} \left\{ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \mid \mathcal{F} \right\} \right\} \to 0. \tag{A.4}$$

Thus, from (A.2) and (A.4) we get

$$\text{Var} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right] = \text{Var} \left\{ \mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right] \right\} + \mathbb{E} \left\{ \text{Var} \left[ \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \right] \right\} \xrightarrow{p} 0. \tag{A.5}$$

Finally, (A.3) and (A.5) together reveal that

$$\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_i, \beta_i) h(\hat{\beta}_{p+i}) \xrightarrow{p} \mathbb{E} \left[ g(\eta_{\alpha' \tau'}(\Pi + \tau' Z), \Pi) \right] \mathbb{E} \left[ h(\eta_{\alpha' \tau'}(\tau' Z)) \right] \as p \to \infty.$$
In the remainder of this subsection, we complete the proof of Lemmas A.2, A.3, and A.4. In the proof of Lemma A.2 we need the following preparatory lemma.

**Lemma A.5.** Let \( \{\xi_{p1}, \xi_{p2}, \ldots, \xi_{pm}\}_{p=1}^{\infty} \) be a triangular array of bounded random variables such that \( \xi_{p1}, \xi_{p2}, \ldots, \xi_{pm} \) are exchangeable for every \( p \) and \( m_p \to \infty \) as \( p \to \infty \). If for a constant \( c \),

\[
\frac{\xi_{p1} + \cdots + \xi_{pm}}{m_p} \overset{p}{\to} c
\]

as \( p \to \infty \), for an arbitrary (deterministic) sequence \( l_p \) satisfying \( l_p \leq m_p \) and \( l_p \to \infty \), we must have

\[
\frac{\xi_{p1} + \cdots + \xi_{pl_p}}{l_p} \overset{p}{\to} c.
\]

**Proof of Lemma A.5.** Fix any \( \epsilon > 0 \). We will show that

\[
\lim_{p \to \infty} \mathbb{P}\left\{ \left| \frac{\xi_{p1} + \cdots + \xi_{pl_p}}{l_p} - c \right| > \epsilon \right\} = 0.
\]

For any \( p \) let \( S_p \) be a random subset of \( \{1, \ldots, m_p\} \) of cardinality \( l_p \), drawn independently of the \( \xi_{pi}'s \). Then by exchangeability, \( \sum_{i=1}^{l_p} \xi_{pi} \) is equal in distribution to \( \sum_{i \in S_p} \xi_{pi} \). Therefore we equivalently need to show that

\[
\lim_{p \to \infty} \mathbb{P}\left\{ \left| \frac{\sum_{i \in S_p} \xi_{pi}}{l_p} - c \right| > \epsilon \right\} = 0.
\]

We trivially have

\[
\lim_{p \to \infty} \mathbb{P}\left\{ \left| \frac{\sum_{i \in S_p} \xi_{pi}}{l_p} - c \right| > \epsilon \right\} \leq \lim_{p \to \infty} \mathbb{P}\left\{ \left| \frac{\sum_{i \in S_p} \xi_{pi}}{l_p} - \frac{\xi_{p1} + \cdots + \xi_{pm}}{m_p} \right| > \epsilon / 2 \right\} + \lim_{p \to \infty} \mathbb{P}\left\{ \left| \frac{\xi_{p1} + \cdots + \xi_{pm}}{m_p} - c \right| > \epsilon / 2 \right\}.
\]

The assumption \( \frac{\xi_{p1} + \cdots + \xi_{pm}}{m_p} \overset{p}{\to} c \) implies that

\[
\lim_{p \to \infty} \mathbb{P}\left\{ \left| \frac{\xi_{p1} + \cdots + \xi_{pm}}{m_p} - c \right| > \epsilon / 2 \right\} = 0.
\]

Next we bound the remaining term. Recall that the \( \xi_{pi}'s \) are bounded, so we can assume \( \xi_{pi} \in [-B, B] \) for some finite \( B > 0 \). We then have

\[
\text{Var} \left( \frac{\sum_{i \in S_p} \xi_{pi}}{l_p} \left| \xi_{p1}, \ldots, \xi_{pm} \right. \right) \leq \frac{4B^2}{l_p},
\]

since sampling uniformly with replacement always has variance no larger than sampling uniformly without replacement, and the \( \xi_{pi}'s \) are bounded. Therefore,

\[
\mathbb{P}\left\{ \left| \frac{\sum_{i \in S_p} \xi_{pi}}{l_p} - \frac{\xi_{p1} + \cdots + \xi_{pm}}{m_p} \right| > \epsilon / 2 \left| \xi_{p1}, \ldots, \xi_{pm} \right. \right\} \leq \frac{4B^2 / l_p}{\epsilon^2 / 4}
\]
almost surely. Marginalizing,
\[
P \left\{ \left| \frac{\sum_{i \in S_p} \xi_{pi}}{l_p} - \frac{\xi_p + \cdots + \xi_{pm_p}}{m_p} \right| > \frac{\epsilon}{2} \right\} \leq \frac{4B^2/l_p}{\epsilon^2/4},
\]
which tends to zero as \( p \to \infty \) since \( \epsilon \) is fixed and \( l_p \to \infty \). This completes the proof.

Now, we are ready to prove Lemma A.2.

Proof of Lemma A.2. It suffices to prove the lemma for any bounded Lipschitz continuous functions. To see this, assume for the moment that
\[
\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_{p+i}) \xrightarrow{P} \mathbb{E} g(\eta_{\alpha'\tau'}(\tau'Z)) \quad (A.6)
\]
if \( g \) is bounded and Lipschitz continuous. Let \( f \) be a continuous function and satisfies \( |f(x)| \leq M \) for all \( x \). We show below that
\[
\frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) \xrightarrow{P} \mathbb{E} f(\eta_{\alpha'\tau'}(\tau'Z)). \quad (A.7)
\]

Let \( \nu > 0 \) be an arbitrary small number. As a consequence of Lemma A.7 presented in Section A.2 below, if \( A \) is sufficiently large, then
\[
\frac{\#\{1 \leq i \leq p : |\hat{\beta}_{p+i}| > A\}}{p} \leq \nu \quad (A.8)
\]
with probability tending to one as \( p \to \infty \). As is clear, one can find a Lipschitz continuous function \( g \) defined on a compact set, for example, \([-A, A]\] that satisfies
\[
|f(x) - g(x)| \leq \nu \quad (A.9)
\]
for all \(-A \leq x \leq A\). We can extend \( g \) to a bounded Lipschitz continuous function defined on \( \mathbb{R} \). This can be done, for example, by setting \( g(x) = 0 \) if \( |x| > A + 1 \) and let \( g \) be linear on \([-A - 1, -A]\) and \([A, A + 1]\). Hence, (A.6) holds for \( g \). Let \( M' \) be an upper bound of \( g \) in the sense that \( |g(x)| \leq M' \) for all \( x \) (we can take \( M' = M + \nu \)). To show (A.7), we first write
\[
\frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) = \frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| \leq A} + \frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| > A}
\]
and
\[
\frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_{p+i}) = \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| \leq A} + \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| > A}.
\]
where the indicator function $1$ takes the value $1$ if the event in the subscript happens and takes the value $0$ otherwise. This gives

$$\left| \frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) - \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_{p+i}) \right| \leq \left| \frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| \leq A} - \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| \leq A} \right|$$

$$+ \left| \frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| > A} - \frac{1}{p} \sum_{i=1}^{p} g(\hat{\beta}_{p+i}) 1_{|\hat{\beta}_{p+i}| > A} \right|$$

$$\leq \frac{1}{p} \sum_{i=1}^{p} (|f(\hat{\beta}_{p+i}) - g(\hat{\beta}_{p+i})| 1_{|\hat{\beta}_{p+i}| \leq A}$$

$$+ \frac{1}{p} \sum_{i=1}^{p} M 1_{|\hat{\beta}_{p+i}| > A} + \frac{1}{p} \sum_{i=1}^{p} M' 1_{|\hat{\beta}_{p+i}| > A}$$

$$\leq \frac{1}{p} \sum_{i=1}^{p} |f(\hat{\beta}_{p+i}) - g(\hat{\beta}_{p+i})| 1_{|\hat{\beta}_{p+i}| \leq A} + \frac{(M + M')\#\{1 \leq i \leq p : |\hat{\beta}_{p+i}| > A\}}{p}$$

$$\leq v + (M + M') v$$

$$= (M + M' + 1)v,$$

where in the second last inequality we use (A.9), and the last inequality follows from (A.8) and thus holds with probability tending to one. Similarly, we can show that the difference between $\mathbb{E}g(\eta_{\alpha'\tau'}(\tau'Z))$ and $\mathbb{E}f(\eta_{\alpha'\tau'}(\tau'Z))$ can be made arbitrarily small if $v$ is small enough. Taking $v \to 0$, therefore, we see that (A.6) implies (A.7).

To conclude the proof of this lemma, therefore, it is sufficient to prove (A.6) for any bounded Lipschitz continuous function $g$. For convenience, we write $f$ in place of $g$ and assume that $f$ is bounded by $M$ in magnitude and is $L$-Lipschitz continuous. Consider the function

$$f_a(x, y) = f(x) \max\{0, 1 - |y|/a\}$$

for $a > 0$. Our first step is to verify that this function is Lipschitz continuous and is, therefore, pseudo-Lipschitz continuous (see the definition in [3]). Writing $x_+$ for $\max\{0, x\}$, we note that

$$|f_a(x, y) - f_a(x', y')| = |f(x)(1 - |y|/a)_+ - f(x')(1 - |y'|/a)_+|$$

$$= |f(x)(1 - |y|/a)_+ - f(x)(1 - |y'|/a)_+ + f(x)(1 - |y'|/a)_+ - f(x')(1 - |y'|/a)_+|$$

$$\leq |f(x)(1 - |y|/a)_+ - f(x)(1 - |y'|/a)_+| + |f(x)(1 - |y'|/a)_+ - f(x')(1 - |y'|/a)_+|$$

$$\leq M|y - y'|/a + L(1 - |y'|/a)_+|x - x'|$$

$$\leq (M/a + L)\|(x, y) - (x', y')\|_2.$$  

This proves that $f_a$ is Lipschitz continuous. From Theorem 1.5 of [3], therefore, we get

$$\frac{1}{2p} \sum_{i=1}^{2p} f_a(\hat{\beta}_i, \hat{\beta}_i) \overset{p}{\to} \mathbb{E} f_a \left( \eta_{\alpha\eta}(\bar{\Pi} + \tau'Z), \bar{\Pi} \right)$$

(A.10)

for any fixed $a > 0$, where the random variable $\bar{\Pi} = \Pi$ with probability $\frac{1}{2}$ and otherwise $\bar{\Pi} = 0$.  

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Now we will take \( a \to 0 \) in the right-hand side of (A.10). Recognizing that \( f_a \left( \eta_{\alpha'\tau'}(\bar{\Pi} + \tau'Z), \bar{\Pi} \right) \to f \left( \eta_{\alpha'\tau'}(\bar{\Pi} + \tau'Z) \right) \) if \( \bar{\Pi} = 0 \) and otherwise \( f_a \left( \eta_{\alpha'\tau'}(\bar{\Pi} + \tau'Z), \bar{\Pi} \right) \to 0 \) as \( a \to 0 \), the boundedness of \( f_a \) allows us to use Lebesgue’s dominated convergence theorem to obtain

\[
\lim_{a \to 0^+} E f_a \left( \eta_{\alpha'\tau'}(\bar{\Pi} + \tau'Z), \bar{\Pi} \right) = \frac{1}{2} E f \left( \eta_{\alpha'\tau'}(\tau'Z) \right) + \frac{1}{2} E f \left( \eta_{\alpha'\tau'}(\tau'Z) \right) - \epsilon \frac{E f \left( \eta_{\alpha'\tau'}(\tau'Z) \right)}{2}
\]

(A.11)

Turning to the left-hand side of (A.10), we use the fact that for any \( c_1 > 0 \), one can find \( c_2 > 0 \) such that

\[
\left| \frac{1}{2p} \sum_{i: \beta_i \neq 0} f_a(\tilde{\beta}_i, \beta_i) \right| \leq c_1
\]

(A.12)

with probability approaching one for each \( a < c_2 \). To see this, note that

\[
\left| \frac{1}{2p} \sum_{i: \beta_i \neq 0} f_a(\tilde{\beta}_i, \beta_i) \right| \leq \frac{1}{2p} \sum_{i: \beta_i \neq 0} |f_a(\tilde{\beta}_i, \beta_i)| \leq \frac{1}{2p} \sum_{i: \beta_i \neq 0} M(1 - |\beta_i|/a)_+
\]

of which the expectation satisfies

\[
E \left[ \frac{1}{2p} \sum_{i: \beta_i \neq 0} M(1 - |\beta_i|/a)_+ \right] = \frac{\epsilon}{2} E [M(1 - |\Pi^*|/a)_+] \leq \frac{M\epsilon}{2} \mathbb{P}(|\Pi^*| < a),
\]

since \( \Pi^* \) places no mass at zero, by definition. This inequality in conjunction with the Markov inequality reveals that (A.12) holds if \( a \) is sufficiently small.

Writing

\[
\frac{1}{2p} \sum_{i=1}^{2p} f_a(\tilde{\beta}_i, \beta_i) = \frac{1}{2p} \sum_{i: \beta_i \neq 0} f_a(\tilde{\beta}_i, \beta_i) + \frac{1}{2p} \sum_{i: \beta_i = 0} f_a(\tilde{\beta}_i)
\]

and taking \( a \to 0 \), we get

\[
\frac{1}{2p} \sum_{1 \leq i \leq 2p: \beta_i = 0} f(\tilde{\beta}_i) \xrightarrow{p} \frac{2 - \epsilon}{2} E f \left( \tau' \eta_{\alpha'}(Z) \right)
\]

from (A.11), (A.10), and (A.12). This is equivalent to

\[
\frac{\sum_{1 \leq i \leq 2p: \beta_i = 0} f(\tilde{\beta}_i)}{\# \{1 \leq i \leq 2p : \beta_i = 0 \}} \xrightarrow{p} E f \left( \tau' \eta_{\alpha'}(Z) \right),
\]

(A.13)

which makes use of the fact that

\[
\frac{\# \{1 \leq i \leq 2p : \beta_i = 0 \}}{2p} \xrightarrow{p} \frac{2 - \epsilon}{2}.
\]

(A.14)
To conclude the proof of this lemma, we apply Lemma \[ \text{A.5} \] to \[ \text{(A.13)} \]. This is done by letting \( m_p = \#\{1 \leq i \leq 2p : \beta_i = 0\} \) and \( \{\xi_{p1}, \xi_{p2}, \ldots, \xi_{pm_p}\} = \{f(\hat{\beta}_i) : \beta_i = 0, 1 \leq i \leq 2p\} \) and \( l_p = p \) and \( \{\xi_{p1}, \xi_{p2}, \ldots, \xi_{pm_p}\} = \{f(\hat{\beta}_i) : \beta_i = 0, p+1 \leq i \leq 2p\} \). For completeness, we remark that the randomness of \( m_p \) does not affect the validity of Lemma \[ \text{A.5} \] due to \[ \text{(A.14)} \]. Thus, we get
\[
\frac{1}{p} \sum_{i=p+1}^{2p} f(\hat{\beta}_i) = \frac{1}{p} \sum_{i=p+1}^{2p} f(\hat{\beta}_i) \xrightarrow{p} \mathbb{E} f(\tau' \eta_{\alpha'}(Z)).
\]
This completes the proof. \( \square \)

**Proof of Lemma \[ \text{A.3} \]** As with Lemma \[ \text{A.2} \] it is sufficient to prove the present lemma for any bounded Lipschitz continuous functions. By Theorem 1.5 of \[ \Pi \], we get
\[
\frac{1}{2p} \sum_{i=1}^{2p} f(\hat{\beta}_i, \beta_i) = \frac{1}{2p} \sum_{i=1}^{2p} f(\hat{\beta}_i, \beta_i) + \frac{1}{2p} \sum_{i=p+1}^{2p} f(\hat{\beta}_i, 0) \xrightarrow{p} \mathbb{E} f(\eta_{\alpha'\tau'}(\Pi + \tau' Z), \Pi).
\]  
\[ \text{(A.15)} \]
Note that the right-hand side can be written as
\[
\mathbb{E} f(\eta_{\alpha'\tau'}(\Pi + \tau' Z), \Pi) = \frac{1}{2} \mathbb{E} f(\eta_{\alpha'\tau'}(\Pi + \tau' Z), \Pi) + \frac{1}{2} \mathbb{E} f(\eta_{\alpha'\tau'}(\tau' Z), 0).
\]  
\[ \text{(A.16)} \]
On the other hand, from Lemma \[ \text{A.2} \] we know
\[
\frac{1}{p} \sum_{i=1}^{2p} f(\hat{\beta}_i, 0) \xrightarrow{p} \mathbb{E} f(\eta_{\alpha'\tau'}(\tau' Z), 0).
\]  
\[ \text{(A.17)} \]
Plugging \[ \text{(A.17)} \] into \[ \text{(A.15)} \] and recognizing \[ \text{(A.16)} \], we get
\[
\frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_i, \beta_i) \xrightarrow{p} \mathbb{E} f(\eta_{\alpha'\tau'}(\Pi + \tau' Z), \Pi).
\]
This completes the proof. \( \square \)

**Proof of Lemma \[ \text{A.4} \]** We have
\[
\text{Var}(A_1 B_{\pi(1)} + \cdots + A_p B_{\pi(p)}) = \sum_{i=1}^{p} \text{Var}(A_i B_{\pi(i)}) + 2 \sum_{i<j} \text{Cov}(A_i B_{\pi(i)}, A_j B_{\pi(j)}).
\]
First, we get
\[
\text{Var}(A_i B_{\pi(i)}) = A_i^2 \text{Var}(B_{\pi(i)}) = \frac{A_i^2 \sum_{l=1}^{p}(B_l - \mathcal{B})^2}{p},
\]
where \( \mathcal{B} = (B_1 + \cdots + B_p)/p \), and
\[
\text{Cov}(A_i B_{\pi(i)}, A_j B_{\pi(j)}) = A_i A_j \text{Cov}(B_{\pi(i)}, B_{\pi(j)})
\]
\[
= A_i A_j \left( \mathbb{E} B_{\pi(i)} B_{\pi(j)} - \mathbb{E} B_{\pi(i)} \mathbb{E} B_{\pi(j)} \right)
\]
\[
= A_i A_j \left( \frac{\sum_{i \neq m} B_l B_m}{p(p-1)} - \frac{(B_1 + \cdots + B_p)^2}{p^2} \right)
\]
\[
= -A_i A_j \sum_{l=1}^{p}(B_l - \mathcal{B})^2 \frac{1}{p(p-1)}.
\]
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Thus, we get
\[
\sum_{i=1}^{p} \text{Var}(A_iB_{\pi(i)}) + 2 \sum_{i<j} \text{Cov}(A_iB_{\pi(i)}, A_jB_{\pi(j)})
\]
\[
= \sum_{i=1}^{p} \frac{A_i^2 \sum_{l=1}^{p} (B_l - \bar{B})^2}{p} - 2 \sum_{i<j} A_i A_j \frac{\sum_{l=1}^{p} (B_l - \bar{B})^2}{p(p-1)}
\]
\[
= \left[ \sum_{i=1}^{p} (B_l - \bar{B})^2 \right] \left[ \sum_{i=1}^{p} \frac{A_i^2}{p} - 2 \sum_{i<j} A_i A_j \frac{1}{p(p-1)} \right]
\]
\[
= \frac{\sum_{i=1}^{p} (B_l - \bar{B})^2}{p-1} \frac{\sum_{i=1}^{p} (A_l - \bar{A})^2}{p-1}
\]
\[
= \left[ \sum_{i=1}^{p} (B_l - \bar{B})^2 \right] \left[ \sum_{i=1}^{p} (A_l - \bar{A})^2 \right]
\]
\[
= \left[ \sum_{i=1}^{p} (B_l - \bar{B})^2 \right] \left[ \sum_{i=1}^{p} (A_l - \bar{A})^2 \right]
\]
\[
= \left[ \sum_{i=1}^{p} (B_l - \bar{B})^2 \right] \left[ \sum_{i=1}^{p} (A_l - \bar{A})^2 \right]
\]

A.2 Proof of Theorem 1

We first prove Theorem 1 for a fixed $\lambda$, followed by a discussion showing that the theorem holds uniformly over $\lambda$ in a bounded range. In addition to Lemma A.1, the proof relies on Lemmas A.6 and A.7, which we state below.

Let $C(\Omega, \mathbb{R})$ denote the class of all real-valued continuous functions defined on a compact Hausdorff space $\Omega$.

**Lemma A.6.** Let $\Omega_1$ and $\Omega_2$ be two compact Hausdorff spaces and $f : \Omega_1 \times \Omega_2 \rightarrow \mathbb{R}$ be a continuous function, then for every $\nu > 0$ there exist a positive integer $m$ and continuous functions $g_1, \ldots, g_m$ on $\Omega_1$ and continuous functions $h_1, \ldots, h_m$ on $\Omega_2$ such that

\[
\sup_{(x_1, x_2) \in \Omega_1 \times \Omega_2} \left| f(x_1, x_2) - \sum_{i=1}^{m} g_i(x_1) h_i(x_2) \right| \leq \nu.
\]

Lemma A.6 serves as an approximation tool for our proof. For information, this lemma follows from the Stone–Weierstrass theorem (see Corollary 11.6 in [9]).

**Lemma A.7.**

\[
\lim_{A \rightarrow \infty} \limsup_{p \rightarrow \infty} \mathbb{E} \left[ \frac{\# \{1 \leq i \leq p : \max(|\hat{\beta}_i|, |\beta_i|, |\hat{\beta}_{p+i}|) > A \}}{p} \right] = 0.
\]

**Proof of Lemma A.7.** Note that we have

\[
\# \{1 \leq i \leq p : \max(|\hat{\beta}_i|, |\beta_i|, |\hat{\beta}_{p+i}|) > A \}
\]
\[
\leq \# \{1 \leq i \leq p : |\hat{\beta}_i| > A \} + \# \{1 \leq i \leq p : |\beta_i| > A \} + \# \{p+1 \leq i \leq 2p : |\hat{\beta}_i| > A \}.
\]

It has been proved in [4, 15] that first, we have

\[
\frac{\# \{1 \leq i \leq p : |\hat{\beta}_i| > A \}}{p} \rightarrow \mathbb{P}(|\eta_{\alpha} \tau' (\Pi + \tau' Z)| > A),
\]

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which tends to 0 as $A \to \infty$. Second,
\[ \frac{\#\{1 \leq i \leq p : |\beta_i| > A\}}{p} \xrightarrow{P} \mathbb{P}(|\Pi| > A), \]
and third, we obtain
\[ \frac{\#\{p + 1 \leq i \leq 2p : |\hat{\beta}_i| > A\}}{p} \xrightarrow{P} \mathbb{P}(|\eta_{\alpha'}(\tau'Z)| > A). \]

Last, note that these fractions are all bounded, so Lebesgue’s dominated convergence theorem can be applied here.

Now we turn to the proof of Theorem [1].

Proof of Theorem [1] with a fixed $\lambda$. Denote by $M$ an upper bound of $f$ in absolute value and let $R > 0$ be a number that will later tend to infinity. It is easy to see that we can construct a continuous function $\tilde{f}$ defined on $\mathbb{R}^3$ such that (1) $f(x) \equiv \tilde{f}(x)$ on $B_R \equiv \{x \in \mathbb{R}^3 : \|x\|_2 \leq R\}$, (2) $|\tilde{f}(x)| \leq M$ for all $x$, and (3) $\lim_{\|x\|_2 \to \infty} \tilde{f}(x)$ exists. This can be done, for example, by letting
\[
\tilde{f}(x) = \begin{cases} f(x), & \text{if } \|x\|_2 \leq R \\ f \left( \frac{Rx}{\|x\|_2} \right) e^{-\|x\|_2 + R}, & \text{otherwise}. \end{cases}
\]

From the three properties of $\tilde{f}$, it is easy to see that this is a continuous function on the product of two compact Hausdorff spaces, $\mathbb{R}^2 \cup \{\infty\}$ and $\mathbb{R} \cup \{\infty\}$. From Lemma [A.6] therefore, we know that there exist continuous functions $g_1, \ldots, g_m$ on $\mathbb{R}^2 \cup \{\infty\}$ and $h_1, \ldots, h_m$ on $\mathbb{R} \cup \{\infty\}$ such that
\[
\sup_{x_1, x_2, x_3} \left| \tilde{f}(x_1, x_2, x_3) - \sum_{l=1}^{m} g_l(x_1, x_2) h_l(x_3) \right| \leq \upsilon 
\]
for any small constant $\upsilon > 0$.

Since $g_l$ and $h_l$ are continuous on the compactification of their domains for each $l$, the two functions must be continuous and bounded on $\mathbb{R}^2$ and $\mathbb{R}$, respectively. Thus, we get
\[
\frac{1}{p} \sum_{i=1}^{p} g_l(\hat{\beta}_i, \beta_i) h_l(\hat{\beta}_{p+i}) \xrightarrow{P} \mathbb{E} \left[ g_l(\eta_{\alpha'}(\Pi + \tau'Z), \Pi) \right] \mathbb{E} \left[ h_l(\eta_{\alpha'}(\tau'Z')) \right]
\]
by Lemma [A.1] where $Z$ and $Z'$ are i.i.d. standard normal random variables. This yields
\[
\frac{1}{p} \sum_{i=1}^{p} \sum_{l=1}^{m} g_l(\hat{\beta}_i, \beta_i) h_l(\hat{\beta}_{p+i}) \xrightarrow{P} \sum_{l=1}^{m} \mathbb{E} \left[ g_l(\eta_{\alpha'}(\Pi + \tau'Z), \Pi) \right] \mathbb{E} \left[ h_l(\eta_{\alpha'}(\tau'Z')) \right]
\]
\[
= \mathbb{E} \left[ \sum_{l=1}^{m} g_l(\eta_{\alpha'}(\Pi + \tau'Z), \Pi) h_l(\eta_{\alpha'}(\tau'Z')) \right].
\]
happens with probability tending to one as \( p \to \infty \).

Next, we consider
\[
\frac{1}{p} \sum_{i=1}^{p} f(\tilde{\beta}_i, \beta_i, \tilde{\beta}_{p+i}) - \frac{1}{p} \sum_{i=1}^{p} \tilde{f}(\tilde{\beta}_i, \beta_i, \tilde{\beta}_{p+i})
\]
and
\[
\mathbb{E} f(\eta_{a',\tau'}(\Pi + \tau'Z), \Pi, \eta_{a',\tau'}(\tau'Z')) - \mathbb{E} \tilde{f}(\eta_{a',\tau'}(\Pi + \tau'Z), \Pi, \eta_{a',\tau'}(\tau'Z')).
\]

Our aim is to show that both displays are small. For the first display, note that
\[
\left| f(\tilde{\beta}_i, \beta_i, \tilde{\beta}_{p+i}) - \tilde{f}(\tilde{\beta}_i, \beta_i, \tilde{\beta}_{p+i}) \right| \leq 2M \mathbb{1}_{\|\beta_i, |\beta_i|, |\tilde{\beta}_{p+i}| > R} \leq 2M \max(|\beta_i|, |\beta_i|, |\tilde{\beta}_{p+i}|) > R/\sqrt{3}.
\]
Taking \( A = R/\sqrt{3} \), we obtain
\[
\left| \frac{1}{p} \sum_{i=1}^{p} [f(\tilde{\beta}_i, \beta_i, \tilde{\beta}_{p+i}) - \tilde{f}(\tilde{\beta}_i, \beta_i, \tilde{\beta}_{p+i})] \right| \leq \frac{2M \# \{1 \leq i \leq p : \max(|\beta_i|, |\beta_i|, |\tilde{\beta}_{p+i}|) > A\}}{p}.
\]
Likewise, we show below that \((A.22)\) can be made arbitrarily small in absolute value. To this end, note that
\[
\mathbb{E} \left[ f(\eta_{a',\tau'}(\Pi + \tau'Z), \Pi, \eta_{a',\tau'}(\tau'Z')) - \tilde{f}(\eta_{a',\tau'}(\Pi + \tau'Z), \Pi, \eta_{a',\tau'}(\tau'Z')) \right]
\leq \mathbb{E} \left[ f(\eta_{a',\tau'}(\Pi + \tau'Z), \Pi, \eta_{a',\tau'}(\tau'Z')) - \tilde{f}(\eta_{a',\tau'}(\Pi + \tau'Z), \Pi, \eta_{a',\tau'}(\tau'Z')) \right]
\leq 2M \mathbb{P} \left( \max(|\eta_{a',\tau'}(\Pi + \tau'Z)|, |\Pi|, |\eta_{a',\tau'}(\tau'Z')|) > A \right).
\]
Finally, from \((A.20), \ (A.23), \ and \ (A.24)\) it follows that the event
\[
\left| \frac{1}{p} \sum_{i=1}^{p} f(\tilde{\beta}_i, \beta_i, \tilde{\beta}_{p+i}) - \mathbb{E} f(\eta_{a',\tau'}(\Pi + \tau'Z), \Pi, \eta_{a',\tau'}(\tau'Z')) \right|
< 3v + \frac{2M \# \{1 \leq i \leq p : \max(|\beta_i|, |\beta_i|, |\tilde{\beta}_{p+i}|) > A\}}{p} + 2M \mathbb{P} \left( \max(|\eta_{a',\tau'}(\Pi + \tau'Z)|, |\Pi|, |\eta_{a',\tau'}(\tau'Z')|) > A \right)
\]
happens with probability tending to one as \( p \to \infty \). Taking \( A \equiv R/\sqrt{3} \to \infty \) followed by letting \( v \to 0 \), Lemma \( A.7 \) shows that
\[
3v + \frac{2M \# \{1 \leq i \leq p : \max(|\beta_i|, |\beta_i|, |\tilde{\beta}_{p+i}|) > A\}}{p} + 2M \mathbb{P} \left( \max(|\eta_{a',\tau'}(\Pi + \tau'Z)|, |\Pi|, |\eta_{a',\tau'}(\tau'Z')|) > A \right)
\]

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can be made arbitrarily small. This reveals that

\[
\frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_i, \beta_i, \hat{\beta}_{p+i}) \xrightarrow{p} \mathbb{E} \left[ f(\eta_{\alpha'\tau'}(\Pi + \tau'Z), \Pi, \eta_{\alpha'\tau'}(\tau'Z')) \right],
\]

thereby completing the proof.

The remaining part of this subsection is devoted to showing that Theorem 1 holds uniformly over all \( \lambda \) in a compact interval of \((0, \infty)\). As with the proof of Lemma A.2, we can assume that \( f \) is bounded and \( L \)-Lipschitz continuous. The uniformity extension is accomplished largely by using Lemma B.2 from [15] (see also [20]).

**Lemma A.8 (Lemma B.2 in [15]).** Fix \( 0 < \lambda_{\text{min}} < \lambda_{\text{max}} \). Then, there exists a constant \( c \) such that for any \( [\lambda^-, \lambda^+] \subset [\lambda_{\text{min}}, \lambda_{\text{max}}] \), the Lasso estimates satisfy

\[
\sup_{\lambda^- \leq \lambda \leq \lambda^+} \left\| \hat{\beta}(\lambda) - \hat{\beta}(\lambda^-) \right\|_2 \leq c \sqrt{(\lambda^+ - \lambda^-) p}
\]

with probability tending to one.

To begin to establish the uniformity in \( \lambda \), let \( \lambda_{\text{min}} = \lambda_0 < \lambda_1 < \cdots < \lambda_m = \lambda_{\text{max}} \) be equally spaced points and set \( \Delta \equiv \lambda_{l+1} - \lambda_l = (\lambda_{\text{max}} - \lambda_{\text{min}})/m \); We will later take \( m \to \infty \). Write

\[
f^\infty(\lambda) = \mathbb{E} f(\eta_{\alpha'\tau'}(\Pi + \tau'Z), \Pi, \eta_{\alpha'\tau'}(\tau'Z')).
\]

It follows from Theorem 1 that

\[
\max_{0 \leq l \leq m} \left| \frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_i(\lambda_l), \beta_i, \hat{\beta}_{p+i}(\lambda_l)) - f^\infty(\lambda_l) \right| \xrightarrow{p} 0. \quad (A.25)
\]

Now, according to Corollary 1.7 from [3], both \( \alpha', \tau' \) are continuous in \( \lambda \) and, therefore, \( f^\infty(\lambda) \) is also continuous on \([\lambda_{\text{min}}, \lambda_{\text{max}}] \). For any constant \( \omega > 0 \), therefore, the uniform continuity of \( f^\infty \) ensures that

\[
|f^\infty(\lambda) - f^\infty(\lambda')| \leq \omega \quad (A.26)
\]
holds for all \( \lambda_{\min} \leq \lambda, \lambda' \leq \lambda_{\max} \) satisfying \(|\lambda - \lambda'| \leq \Delta\) if \( m \) is sufficiently large. Now we consider

\[
\left| \frac{1}{p} \sum_{i=1}^{p} f(\beta_i, \lambda, \beta_i, \beta_{p+i}(\lambda)) - \frac{1}{p} \sum_{i=1}^{p} f(\beta_i^{(\lambda')}, \lambda, \beta_i, \beta_{p+i}(\lambda')) \right| \\
\leq \frac{1}{p} \sum_{i=1}^{p} \left| f(\beta_i, \lambda, \beta_i, \beta_{p+i}(\lambda)) - f(\beta_i^{(\lambda')}, \lambda, \beta_i, \beta_{p+i}(\lambda')) \right| \\
\leq \frac{1}{p} \sum_{i=1}^{p} L \sqrt{(\beta_i - \beta_i^{(\lambda')})^2 + (\beta_i - \beta_i^{(\lambda')})^2} \\
\leq \frac{1}{p} \sum_{i=1}^{p} \left( L |\beta_i - \beta_i^{(\lambda')}| + L |\beta_{p+i}(\lambda) - \beta_{p+i}(\lambda')| \right) \\
= \frac{L}{p} \| \beta(\lambda) - \beta^{(\lambda')} \|_1 \\
\leq \frac{L}{p} \sqrt{2p} \| \beta(\lambda) - \beta^{(\lambda')} \|_2 \\
= \frac{\sqrt{2L}}{\sqrt{p}} \| \beta(\lambda) - \beta^{(\lambda')} \|_2.
\]

Taking \( \lambda' = \lambda_l \) for some \( l = 0, 1, \ldots, m - 1 \) and \( \lambda_l < \lambda < \lambda_{l+1} \), Lemma A.8 ensures that

\[
\sup_{\lambda_l \leq \lambda \leq \lambda_{l+1}} \left| \frac{1}{p} \sum_{i=1}^{p} f(\beta_i, \lambda, \beta_i, \beta_{p+i}(\lambda)) - \frac{1}{p} \sum_{i=1}^{p} f(\beta_i^{(\lambda_l)}, \lambda, \beta_i, \beta_{p+i}(\lambda_l)) \right| \\
\leq \sup_{\lambda_l \leq \lambda \leq \lambda_{l+1}} \frac{\sqrt{2L}}{\sqrt{p}} \| \beta(\lambda) - \beta^{(\lambda_l)} \|_2 \\
\leq \sup_{\lambda_l \leq \lambda \leq \lambda_{l+1}} \frac{\sqrt{2L}}{\sqrt{p}} c \sqrt{(\lambda - \lambda_l)p} \\
= \sqrt{2L} c \sqrt{\frac{\lambda_{\max} - \lambda_{\min}}{m}} \\
= O(1/\sqrt{m})
\]

with probability tending to one. Taking a union bound, we get

\[
\max_{0 \leq l \leq m} \sup_{\lambda_l \leq \lambda \leq \lambda_{l+1}} \left| \frac{1}{p} \sum_{i=1}^{p} f(\beta_i^{(\lambda_l)}, \lambda, \beta_i, \beta_{p+i}(\lambda_l)) - \frac{1}{p} \sum_{i=1}^{p} f(\beta_i(\lambda_t), \beta_i, \beta_{p+i}(\lambda_t)) \right| = O(1/\sqrt{m}) \quad (A.27)
\]

with probability tending to one as \( p \to \infty \).

Now, for any \( \lambda \in [\lambda_{\min}, \lambda_{\max}] \), choose \( l \) such that \( \lambda_l \leq \lambda < \lambda_{l+1} \) (set \( \lambda_{m+1} = \lambda_{\max} + \Delta \)). Then from (A.25), (A.26), and (A.27) we obtain

\[
\left| \frac{1}{p} \sum_{i=1}^{p} f(\beta_i^{(\lambda_l)}, \beta, \beta_{p+i}(\lambda_l)) - f^\infty(\lambda) \right| \\
\leq \left| \frac{1}{p} \sum_{i=1}^{p} f(\beta_i^{(\lambda_l)}, \beta, \beta_{p+i}(\lambda_l)) - \frac{1}{p} \sum_{i=1}^{p} f(\beta_i(\lambda_t), \beta, \beta_{p+i}(\lambda_t)) \right|.
\]
allows us to set \( \lambda \) holds uniformly for all \( \lambda \in [\lambda_{\text{min}}, \lambda_{\text{max}}] \) with probability tending to one. Taking \( m \to \infty \), which allows us to set \( \omega \to 0 \), gives

\[
\sup_{\lambda_{\text{min}} \leq \lambda \leq \lambda_{\text{max}}} \left| \frac{1}{p} \sum_{i=1}^{p} f(\hat{\beta}_i(\lambda), \beta, \hat{\beta}_{p+i}(\lambda)) - f^\infty(\lambda) \right| \overset{p}{\to} 0
\]

as \( p \to \infty \).

### A.3 Proof of Theorem 2

The proof of Theorem 2 presented here applies to not only the LCD statistic used in the knockoffs procedure but, more broadly, any statistic of the form \( W_j(\lambda) = w(\hat{\beta}_j(\lambda), \hat{\beta}_{j+p}(\lambda)) \) where the link function \( w \) is faithful in the sense that it satisfies \( w(u, v) = -w(v, u) \) and \( w(x, c) \to \infty \) as \( |x| \to \infty \) for any fixed \( c \). Our proof below considers \( 0 < q < \frac{1-c}{1+c} \).

Let \( t > 0 \) be the unique value of \( t \) satisfying

\[
\hat{f}_{\text{dp}}(t) = \frac{\mathbb{P}(w(\eta_{\alpha'}(\Pi + \tau'Z), \tau'\eta_{\alpha'}(Z')) \leq -t)}{\mathbb{P}(w(\eta_{\alpha'}(\Pi + \tau'Z), \tau'\eta_{\alpha'}(Z')) \geq t)} = q.
\]

When the prior distribution is \( \Pi_m \), denote by \( \alpha'_m, \tau'_m \) the solution to (3.4) and let \( \hat{t}_m \) be defined as above. Recognizing the growing assumption of \( \Pi_m \) in Definition 3.3, one can show that \( \alpha'_m, \tau'_m \) converge to \( \alpha'_{\infty}, \tau'_{\infty} \) which are the solution to

\[
\tau^2 = \sigma^2 + \frac{\epsilon \tau^2 (1 + \alpha^2)}{\delta} + \frac{2 - \epsilon}{\delta} \mathbb{E} \eta_{\alpha'}(\tau Z)^2
\]

\[
\lambda = \left[ 1 - \frac{\epsilon}{\delta} - \frac{2 - \epsilon}{\delta} \mathbb{P}(|\tau Z| > \alpha \tau) \right] \alpha \tau.
\]

That is, \( \alpha'_m \to \alpha'_{\infty} \) and \( \tau'_m \to \tau'_{\infty} \) as \( m \to \infty \). As a consequence, \( \hat{t}_m \) tends to \( \hat{t}_{\infty} \) as \( m \to \infty \) as well, where the existence of \( \hat{t}_{\infty} \) is ensured by the fact that \( 0 < q < \frac{1-c}{1+c} \).

Following the proof of Lemma A.1 in [15], we can show that \( \text{TPP}(\lambda, \Pi_m, q) \) converges to

\[
\text{tpp}(\lambda, \Pi_m, q) \equiv \mathbb{P}(w(\eta_{\alpha'_m}(\Pi_m + \tau'_m Z), \tau'_m \eta_{\alpha'_m}(Z')) \geq \hat{t}_m | \Pi_m \neq 0)
\]

in probability uniformly over \( \lambda_1 \leq \lambda \leq \lambda_2 \) as \( n \to \infty \), by making use of Theorem 1. Having demonstrated earlier that \( \alpha'_m \) and \( \tau'_m \) converge to constants, the faithfulness of \( w \) and the growing condition of \( \Pi_m \) reveal that

\[
\text{tpp}(\lambda, \Pi_m, q) \to 1.
\]

Moreover, the convergence of the probability \( \text{tpp}(\lambda, \Pi_m, q) \) as a smooth function of \( \lambda \) to its limit 1 is uniform over \( \lambda_1 \leq \lambda \leq \lambda_2 \) as \( m \to \infty \). In particular, we can choose \( m' \) such that

\[
\inf_{\lambda_1 \leq \lambda \leq \lambda_2} \text{tpp}(\lambda, \Pi_m, q) > 1 - \frac{\nu}{2}
\]

(A.28)
for all $m \geq m'$. Furthermore, for any $m$ we can find $n'(m)$ such that

$$\sup_{\lambda_1 \leq \lambda \leq \lambda_2} |TPP(\lambda, \Pi_m, q) - tpp(\lambda, \Pi_m, q)| < \frac{\nu}{2}$$  \hspace{1cm} (A.29)

happens with probability at least $1 - \nu$ when $n \geq n'(m)$. Taken together, (A.28) and (A.29) ensure that, with probability at least $1 - \nu$, we have

$$\inf_{\lambda_1 \leq \lambda \leq \lambda_2} TPP(\lambda, \Pi_m, q) > 1 - \nu$$

for $n \geq n'(m)$ and $m \geq m'$. This concludes the proof.

**B Derivation of the CV-AMP equations**

Denote the minimum value for $\tau$ by

$$\tau_{cv} \equiv \min_{\lambda} \tau(\lambda; (K - 1)\delta/K),$$

and let $\alpha_{cv}$ be the corresponding value for $\alpha$ (so $\alpha_{cv}$ is the solution in $\alpha$ to the first equation in (3.4) when $\tau$ replaced by $\tau_{cv}$). Note that we can characterize $(\alpha_{cv}, \tau_{cv})$ by requiring that for $0 < t < \tau_{cv}$,

$$t^2 = \sigma^2 + \frac{K}{(K - 1)\delta} \mathbb{E} \left[ \eta_{\alpha_{cv}}(\Pi + tZ - \Pi) \right]^2 + \frac{K}{(K - 1)\delta} \mathbb{E} \left[ \eta_{\alpha_{cv}}(tZ) \right]^2$$

does not have a solution in $t$ for $\alpha > \alpha_{\text{min}}$. Therefore, on defining

$$f(u) \equiv \sigma^2 + \frac{K}{(K - 1)\delta} \mathbb{E} \left[ \eta_{\alpha_{cv}}(\Pi + \tau_{cv}Z - \Pi) \right]^2 + \frac{K}{(K - 1)\delta} \mathbb{E} \left[ \eta_{\alpha_{cv}}(\tau_{cv}Z) \right]^2 - \tau_{cv}^2,$$

we are looking to solve

$$\left. \frac{df(u)}{du} \right|_{u=\alpha_{cv}} = 0.$$  \hspace{1cm} (B.1)

It is easy to verify, on the other hand, that

$$\frac{df(u)}{du} = \frac{2\tau_{cv}^2 K}{(K - 1)\delta} \left[ \mathbb{E} [Z + u; \Pi + \tau Z < -\tau u] - \mathbb{E} [Z - u; \Pi + \tau Z > \tau u] - \frac{4\tau_{cv}^2 K}{(K - 1)\delta} \left[ \phi(u) - u \Phi(-u) \right] \right].$$

Imposing now (B.1), we get the equation system

$$\tau_{cv}^2 = \sigma^2 + \frac{K}{(K - 1)\delta} \mathbb{E} \left[ \eta_{\alpha_{cv}}(\Pi + \tau_{cv}Z - \Pi) \right]^2 + \frac{K}{(K - 1)\delta} \mathbb{E} \left[ \eta_{\alpha_{cv}}(\tau_{cv}Z) \right]^2$$

$$\frac{2\tau_{cv}^2 K}{(K - 1)\delta} \left[ \mathbb{E} [Z + \alpha_{cv}; \Pi + \tau_{cv}Z < -\tau_{cv}\alpha_{cv}] - \mathbb{E} [Z - \alpha_{cv}; \Pi + \tau_{cv}Z > \tau_{cv}\alpha_{cv}] \right]$$

$$- \frac{4\tau_{cv}^2 K}{(K - 1)\delta} \left[ \phi(\alpha_{cv}) - \alpha_{cv} \Phi(-\alpha_{cv}) \right] = 0,$$

which simplifies to (4.2).