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SUPPLEMENT TO "CONTROLLING THE FALSE DISCOVERY RATE VIA KNOCKOFFS"

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APPENDIX A: PROOFS

This section gives a proof of Theorem 3 for both procedures. We work with $K = \{1, \ldots, m\}$ as the proof for an arbitrary $K \subsetneq \{1, \ldots, m\}$ is identical. Throughout this section, we assume the conditions of Theorem 3, namely that the null p-values are iid, satisfy $p_j \geq \mathsf{Unif}[0, 1]$, and are independent from the non-nulls.

A.1. Martingales. In [1], the authors offered a new and elegant proof of the FDR controlling property of the BHq procedure based on a martingale argument. While our argument is different, it also uses martingale theory.

LEMMA 1 (Martingale process). *For $k = m, m-1, \ldots, 1, 0$, put $V^+(k) = \#\{\text{null } j : 1 \leq j \leq k, p_j \leq c\}$ and $V^-(k) = \#\{\text{null } j : 1 \leq j \leq k, p_j > c\}$ with the convention that $V^{\pm}(0) = 0$. Let $\mathcal{F}_k$ be the filtration defined by knowing all the non-null p-values, as well as $V^{\pm}(k')$ for all $k' \geq k$. Then the process*

$$M(k) = \frac{V^+(k)}{1 + V^-(k)}$$

is a super-martingale running backward in time with respect to $\mathcal{F}_k$. For any fixed q, $\hat{k}$ defined as in either sequential testing procedure is a stopping time, and as a consequence

$$\mathbb{E}\left[\frac{\#\{\text{null } j \leq \hat{k} : p_j \leq c\}}{1 + \#\{\text{null } j \leq \hat{k} : p_j > c\}}\right] \leq \frac{c}{1-c}. \tag{A.1}$$

PROOF. Note that the filtration $\mathcal{F}_k$ informs us about whether k is null or not, since the non-null process is known exactly. On the one hand, if k is non-null, then $M(k-1) = M(k)$. On the other, if k is null, then

$$M(k-1) = \frac{V^+(k) - I}{1 + V^-(k) - (1 - I)} = \frac{V^+(k) - I}{(V^-(k) + I) \vee 1}, \qquad \text{where } I = \mathbb{1}_{p_k \leq c}.$$

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The event $\mathcal{F}_k$ gives no further knowledge about I, and it follows from the exchangeability property of the nulls—they are i.i.d. and thus exchangeable—that $\mathbb{P}\{I = 1\} = V^+(k)/(V^+(k) + V^-(k))$. Thus in the case where k is null,

$$\mathbb{E}\left[M(k-1)|\mathcal{F}_k\right] = \frac{1}{V^+(k)+V^-(k)}\left[V_+(k)\frac{V^+(k)-1}{V^-(k)+1} + V^-(k)\frac{V^+(k)}{V^-(k)\vee 1}\right]$$
$$= \begin{cases} \frac{V^+(k)}{1+V^-(k)}, & V^-(k) > 0, \\ V^+(k) - 1, & V^-(k) = 0. \end{cases}$$

In summary,

$$\mathbb{E}\left[M(k-1)|\mathcal{F}_k\right] = \begin{cases} M(k), & k \text{ non null}, \\ M(k), & k \text{ null and } V^-(k) > 0, \\ M(k) - 1, & k \text{ null and } V^-(k) = 0, \end{cases}$$

which shows that $\mathbb{E}\left[M(k-1)|\mathcal{F}_k\right] \leq M(k)$. This establishes the super-martingale property.

Now $\hat{k}$ is a stopping time with respect to the backward filtration $\{\mathcal{F}_k\}$ since $\{\hat{k} \geq k\} \in \mathcal{F}_k$. The last assertion (A.1) follows from the optimal stopping time theorem for super-martingales which states that

$$\mathbb{E}M(\hat{k}) \leq \mathbb{E}M(m) = \mathbb{E}\left[\frac{\#\{\text{null } j : p_j \leq c\}}{1 + \#\{\text{null } j : p_j > c\}}\right].$$

Set $X = \#\{\text{null } j : p_j \leq c\}$. The independence of the nulls together with the stochastic dominance $p_j \overset{d}{\geq} \mathsf{Unif}[0,1]$ valid for all nulls imply that $X \overset{d}{\leq} \mathsf{Binomial}(N, c)$, where $Y \sim \mathsf{Binomial}(N, c)$, and N is the total number of nulls. Further, since the function $x \mapsto x/(1 + N - x)$ is nondecreasing, we have

$$\mathbb{E}\left[\frac{X}{1+N-X}\right] \leq \mathbb{E}\left[\frac{Y}{1+N-Y}\right] \leq \frac{c}{1-c},$$

where the last step is proved as follows:

$$\begin{aligned}
\mathbb{E}\left[\frac{Y}{1+N-Y}\right] &= \mathbb{E}\left[\frac{Y}{1+N-Y}\cdot \mathbb{1}_{Y>0}\right]\\
&= \sum_{i=1}^{N} \mathbb{P}\left\{Y=i\right\}\cdot \frac{i}{1+N-i}\\
&= \sum_{i=1}^{N} c^i(1-c)^{N-i}\cdot \frac{N!}{i!(N-i)!}\cdot \frac{i}{1+N-i}\\
&= \frac{c}{1-c}\sum_{i=1}^{N} c^{i-1}(1-c)^{N-i+1}\cdot \frac{N!}{(i-1)!(N-i+1)!}\\
&= \frac{c}{1-c}\sum_{i=1}^{N} \mathbb{P}\left\{Y=i-1\right\}\\
&\leq \frac{c}{1-c}.
\end{aligned}$$

□

The proof of Lemma 4 establishes that $\mathbb{E}\left[M(k-1)|\mathcal{F}_k\right] = M(k)$ unless $V^-(k) = 0$. If $V^-(\hat{k}) > 0$, then we have not yet reached the part of the supermartingale where the expectation may decrease. In turn, this means that if there are several false positives in our set of discoveries, then $V^-(\hat{k})$ will probably be nonzero. Therefore, we can expect to have $\mathbb{E}\left[M(\hat{k})\right] \approx \mathbb{E}\left[M(m)\right] \approx 1$, except perhaps in cases when there are very few discoveries.

A.2. Proof of Theorem 3 for Selective SeqStep. Recall that $V = \#\{\text{null } j \leq \hat{k} : p_j \leq c\}$ and $R = \#\{j \leq \hat{k} : p_j \leq c\}$. For Selective SeqStep+, write $\hat{k} = \hat{k}_1$, and proceed as in Section 2.4:

$$\begin{aligned}
&\mathbb{E}\left[\frac{V}{R\vee 1}\right] = \mathbb{E}\left[\frac{V}{R\vee 1}\cdot \mathbb{1}_{\hat{k}>0}\right]\\
&= \mathbb{E}\left[\frac{\#\{\text{null } j\leq \hat{k} : p_j\leq c\}}{1+\#\{\text{null } j\leq \hat{k} : p_j > c\}}\cdot\left(\frac{1+\#\{\text{null } j\leq \hat{k} : p_j > c\}}{\#\{j\leq \hat{k} : p_j\leq c\}\vee 1}\cdot \mathbb{1}_{\hat{k}>0}\right)\right]\\
&\leq \mathbb{E}\left[\frac{\#\{\text{null } j\leq \hat{k} : p_j\leq c\}}{1+\#\{\text{null } j\leq \hat{k} : p_j > c\}}\right]\cdot\frac{1-c}{c}\cdot q\\
&\leq q,
\end{aligned}$$

where the first inequality applies the definition of $\hat{k}$ to bound the quantity in parentheses, and the second inequality applies (A.1) from Lemma 1. Similarly, consider

Selective SeqStep and set $\hat{k} = \hat{k}_0$. Then

$$\begin{aligned}
\mathbb{E}\left[\frac{V}{\frac{c}{1-c}q^{-1}+R}\right] &= \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1+\#\{\text{null } j \le \hat{k} : p_j > c\}} \cdot \frac{1+\#\{\text{null } j \le \hat{k} : p_j > c\}}{\frac{c}{1-c}q^{-1}+R}\right] \\
&\le \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1+\#\{\text{null } j \le \hat{k} : p_j > c\}} \cdot \frac{1+\frac{1-c}{c}\cdot qR}{\frac{c}{1-c}+qR}\right] \cdot q \\
&= \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1+\#\{\text{null } j \le \hat{k} : p_j > c\}}\right] \cdot \frac{1-c}{c} \cdot q \\
&\le q,
\end{aligned}$$

where the first inequality applies the definition of $\hat{k}$, which gives $\#\{\text{null } j \le \hat{k} : p_j > c\} \le \frac{1-c}{c} \cdot qR$, and the last inequality applies Lemma 1. This proves Theorems 1 and 2.

A.3. Proof of Theorem 3 for SeqStep. Consider SeqStep+ first and set $\hat{k} = \hat{k}_1$. Then with

$$\begin{aligned}
\mathbb{E}\left[\frac{V}{R \vee 1}\right] &= \mathbb{E}\left[\frac{V}{R \vee 1} \cdot \mathbb{1}_{\hat{k}>0}\right] = \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k}\}}{\hat{k} \vee 1} \cdot \mathbb{1}_{\hat{k}>0}\right], \\
\text{FDP}_+(\hat{k}) &= \frac{1+\#\{\text{null } j \le \hat{k}\}}{1+\hat{k}},
\end{aligned}$$

we have

$$\begin{aligned}
&\mathbb{E}\left[\frac{V}{R \vee 1}\right] \le \mathbb{E}\left[\frac{1+\#\{\text{null } j \le \hat{k}\}}{1+\hat{k}} \cdot \mathbb{1}_{\hat{k}>0}\right] \\
&= \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1+\hat{k}} \cdot \mathbb{1}_{\hat{k}>0}\right] + \mathbb{E}\left[\frac{1+\#\{\text{null } j \le \hat{k} : p_j > c\}}{1+\hat{k}} \cdot \mathbb{1}_{\hat{k}>0}\right] \\
&= \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1+\#\{\text{null } j \le \hat{k} : p_j > c\}} \cdot \text{FDP}_+(\hat{k}) \cdot \mathbb{1}_{\hat{k}>0}\right] + \mathbb{E}\left[\text{FDP}_+(\hat{k}) \cdot \mathbb{1}_{\hat{k}>0}\right] \\
&\le \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1+\#\{\text{null } j \le \hat{k} : p_j > c\}}\right] \cdot (1-c) \cdot q + (1-c) \cdot q \\
&\le \frac{c}{1-c} \cdot (1-c) \cdot q + (1-c) \cdot q = q,
\end{aligned}$$

where again the next-to-last inequality applies the definition of $\hat{k}$ and the last inequality applies Lemma 1. Moving to SeqStep and setting $\hat{k} = \hat{k}_0$, write

$$\begin{aligned}
\mathbb{E}\left[\frac{V}{\frac{1}{1-c}q^{-1} + R}\right] &= \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k}\}}{\frac{1}{1-c}q^{-1} + \hat{k}}\right] \\
&= \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{\frac{1}{1-c}q^{-1} + \hat{k}}\right] + \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j > c\}}{\frac{1}{1-c}q^{-1} + \hat{k}}\right] \\
&= \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1 + \#\{\text{null } j \le \hat{k} : p_j > c\}} \cdot \frac{1 + \#\{\text{null } j \le \hat{k} : p_j > c\}}{\frac{1}{1-c}q^{-1} + \hat{k}}\right] \\
&\qquad + \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j > c\}}{\frac{1}{1-c}q^{-1} + \hat{k}}\right].
\end{aligned}$$

This quantity can be bounded by

$$\begin{aligned}
&\mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1 + \#\{\text{null } j \le \hat{k} : p_j > c\}} \cdot \frac{1 + (1-c)\cdot q\hat{k}}{\frac{1}{1-c}q^{-1} + \hat{k}}\right] + \mathbb{E}\left[\frac{(1-c)\cdot q\hat{k}}{\frac{1}{1-c}q^{-1} + \hat{k}}\right] \\
&\le \mathbb{E}\left[\frac{\#\{\text{null } j \le \hat{k} : p_j \le c\}}{1 + \#\{\text{null } j \le \hat{k} : p_j > c\}}\right] \cdot (1-c)\cdot q + (1-c)\cdot q \\
&\le \frac{c}{1-c} \cdot (1-c)\cdot q + (1-c)\cdot q = q,
\end{aligned}$$

where once more the first inequality applies the definition of $\hat{k}$ and the last inequality applies Lemma 1.

APPENDIX B: COMPARING KNOCKOFF WITH BHQ IN THE ORTHOGONAL DESIGN SETTING

Here we sketch a theoretical explanation for the different behaviors of the knockoff and BHq methods, to supplement the empirical comparison shown in Section 3.4 of the main paper. In order to get independent statistics, we work with a $2p \times p$ orthogonal design $\boldsymbol{X}$ and set the noise level $\sigma = 1$ without loss of generality. In this setting, $\boldsymbol{X}^\top \boldsymbol{y} := \boldsymbol{\beta} + \boldsymbol{z} \sim \mathcal{N}(\boldsymbol{\beta}, \mathbf{I})$ is the maximum likelihood estimate for the regression coefficients. Recall that the BHq procedure selects variables $\boldsymbol{X}_j$ with $|\boldsymbol{X}_j^\top \boldsymbol{y}| \ge T$ and

$$T = \min\left\{t : t = +\infty \text{ or } \frac{p \cdot \mathbb{P}\left\{|\mathcal{N}(0,1)| \ge t\right\}}{\#\{j : |\boldsymbol{X}_j^\top \boldsymbol{y}| = |\beta_j + z_j| \ge t\}} \le q\right\}, \tag{B.1}$$

where the fraction above is of course the estimate of $\mathsf{FDP}(t)$. In fact, the number of null features whose statistic exceeds t will be roughly $\pi_0 p \cdot \mathbb{P}\left\{|\mathcal{N}(0,1)| \ge t\right\}$

(since $\pi_0 p$ is the total number of null features), and so the fraction appearing in (B.1) above overestimates $\mathsf{FDP}(t)$ by a factor of $(\pi_0)^{-1}$, leading to FDR control at the level $\pi_0 q$ rather than at the nominal level q.

Next we study the behavior of the knockoff+ procedure in the same setting. By construction, both the equi-correlated and the SDP constructions must obey $\tilde{\boldsymbol{X}}^\top \boldsymbol{X} = \mathbf{0}$ and $\tilde{\boldsymbol{X}}^\top \tilde{\boldsymbol{X}} = \mathbf{I}$. It follows that $\tilde{\boldsymbol{X}}^\top \boldsymbol{y} := \boldsymbol{z}'$ is distributed as $\mathcal{N}(\mathbf{0}, \mathbf{I})$ and is independent from $\boldsymbol{X}^\top \boldsymbol{y}$. Hence, our method specialized to (1.7) yields test statistics of the form

$$W_j = |\beta_j + z_j| \vee |z_j'| \cdot \mathrm{sign}(|\beta_j + z_j| - |z_j'|),$$

and our estimated knockoff+ FDP is equal to

$$\widehat{\mathsf{FDP}}(t) = \frac{1 + \#\{j : |z_j'| \geq t \text{ and } |z_j'| > |\beta_j + z_j|\}}{\#\{j : |\beta_j + z_j| \geq t \text{ and } |\beta_j + z_j| > |z_j'|\}}. \tag{B.2}$$

Now we consider the behavior of this estimated FDP under varying signal magnitude levels. Since there are $\pi_0 p$ null features, and since $|\beta_j| = A$ for the non-nulls, the expected value of the numerator in (B.2) is given by

$$1 + \pi_0 p \cdot \mathbb{P}\left\{|z'| \geq t \text{ and } |z'| > |z|\right\} + (1 - \pi_0) p \cdot \mathbb{P}\left\{|z'| \geq t \text{ and } |z'| > |A + z|\right\}$$

equal to

$$1 + \underbrace{\pi_0 p \cdot \mathbb{P}\{|z| \geq t\}\left(1 - \frac{1}{2}\mathbb{P}\{|z| \geq t\}\right)}_{\text{(Term 1)}} + \underbrace{(1 - \pi_0) p \cdot \mathbb{P}\left\{|z'| \geq t \text{ and } |z'| > |A + z|\right\}}_{\text{(Term 2)}}. \tag{B.3}$$

Consider a large value t. When signal amplitude is high, e.g. $A = 4$, then (Term 1) is the dominant term above, and is roughly equal to $\pi_0 p \cdot \mathbb{P}\{|\mathcal{N}(0,1)| \geq t\}$. In this regime, we see that our procedure resembles BHq (B.1) but with a numerator adjusted to $\pi_0 p \cdot \mathbb{P}\{|\mathcal{N}(0,1)| \geq t\}$ so that it controls the FDR nearly at the nominal level q, instead of $\pi_0 q$.

In contrast, if we consider a weak signal signal magnitude such as $A = 1$, then (Term 2) is no longer vanishing in (B.3) above—that is, the numerator in our FDP estimate may be inadvertently counting non-null features. (In the notation of Section 1.2, we may have non-null j where $W_j < 0$, due to the weakness of the signal.) In this setting, the resulting FDR of the knockoff+ method is conservative, i.e. lower than the nominal level q. However, there is no power loss relative to BHq (see Figure 6); in this low-signal regime, the distribution of the non-null statistics is very close to the null distribution and one simply cannot get any power while controlling a type I error.

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