TOWARDS “SIMULTANEOUS SELECTIVE INFERENCE”:
POST HOC BOUNDS ON THE FALSE DISCOVERY PROPORTION

BY EUGENE KATSEVICH∗† AND AADITYA RAMDAS‡

Stanford University† and Carnegie Mellon University‡

The false discovery rate (FDR) is a popular error criterion for multiple testing, but it has been criticized for lacking flexibility. A target FDR level \( q \) must be set in advance, and the resulting rejection set cannot be contracted or expanded without invalidating FDR control. In exploratory settings, it is desirable to allow the experimenter more freedom to choose a rejection set, while still preserving some Type-I error guarantees. In this paper, we show that the entire path of rejection sets considered by a variety of existing FDR procedures (like BH, knockoffs, and many others) can be endowed with simultaneous high-probability bounds on FDP. The path can be defined based on either the p-values themselves, side information, or a combination of the two. FDR procedures maintain an estimate of FDP for each rejection set on the path, stopping when this estimate exceeds \( q \). We show that inflating this FDP estimate by a small, explicit, multiplicative constant bounds the FDP with high probability across the entire path. These results allow the scientist to spot one or more suitable rejection sets (select post hoc on the algorithm’s trajectory) as they wish, for example by picking a data-dependent size or error level, after examining the FDP bounds for the whole path, and still get a valid high probability FDP bound on the chosen set. Bounding the FDP simultaneously for a selected path of rejection sets (simultaneous selective inference) can be a fruitful middle ground between fully simultaneous inference (guarantees for all possible rejection sets), and fully selective inference (guarantees only for one rejection set).

1. Introduction. The false discovery rate (FDR) of Benjamini and Hochberg (1995) is a popular Type-I error criterion for multiple testing problems. Given a set of hypotheses \( H_1, \ldots, H_n \) (which we identify with \( [n] \equiv \{1, \ldots, n\} \)), the false discovery proportion of a set \( \mathcal{R} \subseteq [n] \) is defined

\[
FDP(\mathcal{R}) \equiv \frac{|\mathcal{R} \cap \mathcal{H}_0|}{|\mathcal{R}|} \equiv \frac{V}{R},
\]

∗E.K.’s work was supported by the Fannie and John Hertz Foundation.

Keywords and phrases: false discovery rate, FDR, multiple testing, post hoc confidence bounds, false discovery exceedance, FDX, simultaneous selective inference, spotting, uniform martingale concentration
where \( \mathcal{H}_0 \subseteq [n] \) is the set of nulls and \( \text{FDP}(\mathcal{R}) \equiv 0 \) when \( \mathcal{R} = \emptyset \) by convention (we use the \( \equiv \) symbol for definitions). Given a multiple testing procedure mapping a set of p-values \( p_1, \ldots, p_n \) to a rejection set \( \mathcal{R}^* \subseteq [n] \), the false discovery rate of this procedure is defined as the expected FDP of the rejection set: \( \text{FDR} \equiv \mathbb{E}[\text{FDP}(\mathcal{R}^*)] \). Despite the popularity of this criterion, the FDR is not without its pitfalls; we describe one of these in the next section.

1.1. Criticism of the FDR, and alternatives. Usually, a target level \( q \) is set in advance, and a rejection set \( \mathcal{R}^* \) is sought such that \( \text{FDR} \leq q \). Storey (2002) points out that this practice derives from traditional multiple testing methods like the family-wise error rate (FWER), where the probability of making any false rejections is bounded by a pre-defined constant \( \alpha \). However, Storey argues that “Because FWER measures the probability of making one or more type I error, which is essentially a 0–1 event, we can set the rate a priori at which this should occur. False discovery rates, in contrast, are more of an exploratory tool. For example, suppose that we are testing 1000 hypotheses and decide beforehand to control FDR at level 5%. Whether this was an appropriate choice largely depends on the number of hypotheses that are rejected. If 100 hypotheses are rejected, then clearly this was a good choice. If only two hypotheses are rejected, then clearly this was a less useful choice.”

Storey’s point is that we are looking for a large rejection set with a small FDP. However, this trade-off can play out differently in different data sets, based on how much signal there is in the data. Therefore, it is somewhat limiting to choose an arbitrary FDR threshold before even seeing the data. Goeman and Solari (2011) (GS), as well as earlier authors (Troendle, 2000; Finner and Roters, 2001), argue eloquently that this inflexibility of the FDR control paradigm clashes with the practice of exploratory data analysis, where domain knowledge and intuition are coupled with the data to choose a “good” rejection set. Importantly, moving to the more conservative false discovery exceedance (FDX) control (for \( \gamma \in (0, 1) \), FDX \( \equiv \Pr(\text{FDP} > \gamma) \)) does not provide any additional flexibility.

To remedy this issue, GS propose a method to obtain FDP upper bounds \( \text{FDP}(\mathcal{R}) \) that hold uniformly across all sets \( \mathcal{R} \) with high-probability:

\[
\Pr\{\text{FDP}(\mathcal{R}) \leq \text{FDP}(\mathcal{R}) \text{ for all } \mathcal{R} \subseteq [n]\} \geq 1 - \alpha.
\]

Such bounds allow the scientist to inspect a “menu” of pairs (\( \mathcal{R}, \text{FDP}(\mathcal{R}) \)) and freely choose the rejection set \( \mathcal{R}^* \). Given the simultaneous nature of statement (2), the upper bound on FDP continues to hold on the chosen set
despite the data-dependent decision made by the user:

\[
\begin{align*}
\Pr\{ \text{FDP}(R^*) \leq \text{FDP}(R) \} & \geq \\
\Pr\{ \text{FDP}(R) \leq \text{FDP}(R) \text{ for all } R \subseteq [n] \} & \geq 1 - \alpha.
\end{align*}
\]

For this reason, bounds like statement (2) are called post hoc bounds. We discuss GS and other related work (Genovese and Wasserman, 2004, 2006; Meinshausen and Rice, 2006; Blanchard, Neuvial and Roquain, 2017) in detail in Section 7.

Therefore, simultaneous inference reconciles rigorous Type-I error guarantees with data exploration. However, this kind of inference may be computationally and statistically costly. Computationally, procedures like GS’s can take exponential time due to their reliance on closed testing, unless “shortcuts” are available in special cases (Goeman and Solari, 2011; Meijer et al., 2017; Dobriban, 2018). Statistically, simultaneous high-probability bounds on the FDP of all \(2^n\) subsets can be conservative.

On the other hand, Storey (2002) proposed the q-value as an exploratory tool to overcome the necessity to set an FDR target level in advance. For any fixed rejection region (say defined by a fixed p-value cutoff \(t\)), the (positive) false discovery rate attached to that region can be estimated. The q-value for a given p-value cutoff \(t\) is then defined as the minimum pFDR estimate attached to any p-value cutoff \(t' \geq t\). While the q-value is a useful exploratory tool, it is rooted in the concept of a fixed rejection region and thus does quite provide rigorous high-probability bounds for rejection sets chosen based on the data. In this paper, we demonstrate that FDP can be bounded without fixing either rejection regions or significance levels in advance.

This paper is about a middle ground between fully selective and fully simultaneous inference, attempting to get the best of both approaches, while addressing their criticisms. We term this “simultaneous selective” inference, because it results in a guarantee that is “simultaneous over a selected path”; we spend Section 2 clarifying what these phrases mean, and then outline our contributions. We state our main results in Section 3, inspect these bounds in Section 4, and prove a key lemma underlying their proofs in Section 5. We then compare our results with prior work in multiple testing and simultaneous inference (Sections 6 and 7) and conclude the paper in Section 8. The supplementary materials contain proofs of our results as well as supplementary discussion.

2. What is “simultaneous selective” inference?. In this paper, we provide a means to obtain simultaneous upper bounds on the FDP of a selected path of candidate rejection sets. In this section, we precisely describe this construction and its utility.
2.1. Simultaneous selective inference. A path or trajectory \( \Pi \) is a nested sequence of \( n \) potential rejection sets:

\[ \text{Path } \Pi \equiv (R_0, \ldots, R_n) \text{ such that } \emptyset \equiv R_0 \subseteq R_1 \subseteq \cdots \subseteq R_n \subseteq [n]. \]

The path is constructed based on the p-values \( P \) (and auxiliary side information) via a “path-selection algorithm” \( \pi \):

\[ \text{Path-selection algorithm } \pi : P \mapsto \Pi, \]

designed to encourage sets on the path to contain many non-nulls. Simultaneous selective inference relies on simultaneous upper bounds \( \text{FDP}(R) \) on \( \text{FDP}(R) \) for each \( R \in \Pi \):

\[ \Pr\{ \text{FDP}(R) \leq \text{FDP}(R) \text{ for all } R \in \Pi \} \geq 1 - \alpha. \]

The guarantee (6) allows the scientist to explore the menu of pairs \( (R, \text{FDP}(R)) \) for \( R \in \Pi \) and spot a set \( R^* \) whose content and FDP bound is to her liking, where to spot is to Select Post hoc On the Trajectory of the algorithm. The FDP bound of this set will remain valid despite this data-dependent (i.e. post hoc) analysis decision, by the same reasoning as (3). Therefore, it provides an alternate solution to flexibility issue raised by Storey, GS, and others.

Compare the simultaneous selective guarantee (6) to the fully simultaneous guarantee (2). The difference is that the former reduces the menu of possible rejection sets from all \( 2^n \) subsets to a path of \( n \) sets. At the price of a smaller menu of candidate rejection sets, we demonstrate below that simultaneous selective inference can provide less conservative bounds than simultaneous inference.

On the other hand, compare simultaneous selective inference with “fully selective inference,” represented by traditional multiple testing procedures, such as FDR methods guaranteeing for a pre-selected \( q \) that

\[ \mathbb{E}[\text{FDP}(R^*)] \leq q; \]

or FDX methods guaranteeing for preselected \( \gamma, \alpha \) that

\[ \Pr\{ \text{FDP}(R^*) > \gamma \} \leq \alpha. \]

These guarantees are fully selective because they hold only for the particular selected set \( R^* \). Most multiple testing methods can be seen as (1) constructing a path \( \Pi \) and then (2) using a pre-defined rule to choose \( R^* \in \Pi \). Note that simultaneous selective inference has the same first step, but the choice of \( R^* \) from \( \Pi \) is left to the user instead of to a pre-defined rule. This provides the extra flexibility that Storey and GS argue for while preserving a rigorous Type-I error guarantee.
2.2. An explicit example. Perhaps the most common path construction algorithm is to sort hypotheses via p-value\(^1\). Formally if

\[
\sigma(i) \text{ is the index of the } i\text{-th smallest p-value},
\]

then define \(\pi_{\text{sort}} : \mathcal{P} \mapsto \Pi_{\text{sort}}\), where

\[
\Pi_{\text{sort}} \equiv (\mathcal{R}_0, \ldots, \mathcal{R}_n) \text{ such that } \mathcal{R}_k \equiv \{\sigma(1), \ldots, \sigma(k)\}.
\]

We prove in this paper that for \(\Pi_{\text{sort}}\), the uniform bound (6) holds with \(\alpha = 0.1\) for

\[
\text{FDP}(\mathcal{R}_k) \equiv \frac{1.93 \cdot (1 + n \cdot p(k))}{|\mathcal{R}_k|}.
\]

Many traditional multiple testing methods use \(\Pi_{\text{sort}}\) as well, each employing a different rule to select \(\mathcal{R}^*\) from \(\Pi_{\text{sort}}\). As one example, Storey (2002) showed that if we define

\[
\hat{\text{FDP}}(\mathcal{R}_k) \equiv \frac{n \cdot p(k)}{|\mathcal{R}_k|},
\]

then the BH method chooses \(\mathcal{R}^* = \mathcal{R}_{k^*}\), where

\[
k^* \equiv \max\{k : \hat{\text{FDP}}(\mathcal{R}_k) \leq q\}.
\]

The user cannot change \(q\) or change the procedure after observing \(\mathcal{R}_{k^*}\) (for example on receiving a set much smaller or larger than they hoped for). However, our uniform bound (6) not only provides a posthoc diagnosis for such an \(\mathcal{R}_{k^*}\), but it also allows the user to pick any other set from \(\Pi_{\text{sort}}\).

Figure 1 illustrates this bound for a toy synthetic example with \(n = 2500\) hypotheses. Of these, 25 are non-null; ten non-nulls have stronger signals with test statistics equal to 3.5 and fifteen have weaker signals with test statistics equal to 3. Null test statistics are drawn from \(N(0, 1)\), and one-sided p-values are then found with respect to this distribution. The bound (9) is depicted in magenta, while the estimate (10) is in red, the ground truth FDP is in black, and the GS bound (based on the Simes local test and computed using the \texttt{cherry} package in \texttt{R}) is in blue.

This figure illustrates selective inference (BH), simultaneous inference (GS), and simultaneous selective inference. With \(q = 0.1\), BH stops where

\(^1\)This is the path used by step-up methods like the BH procedure (Benjamini and Hochberg, 1995), the step-down procedure by Benjamini and Liu (1999), the Storey-BH procedure by Storey (2002) and several other stepwise methods.
0.0
0.2
0.4
0.6
0.8
1.0
1 10 100 1000
Hypothesis Index
False Discovery Proportion
BH FDP estimate FDP bound (Spotting) FDP bound (GS) True FDP

Fig 1. Spotting on the BH path. Based on the red FDP estimate and magenta FDP bound, users may choose any rejection set they like on the path. Point A is the BH rejection set ($q = 0.1$), but B and C might be more attractive options. In this case, our spotting bound is tighter than GS’s simultaneous bound (in blue) along the relevant part of the path.

$\hat{FDP}$ meets the dotted horizontal line at $q = 0.1$ (indicated as the red point labeled “A”), rejecting 11 hypotheses. Our result (6)—with $\hat{FDP}$ defined as in equation (9)—provides extra diagnostic information that the FDP of the BH rejection set can confidently be bounded above by 0.36. We see this from point A on the magenta $\hat{FDP}$ curve. Furthermore, this curve can also be used prescriptively. We see that removing the least significant hypothesis from set A decreases the FDP bound to 0.3, suggesting that the point B on the curve represents a purer set. On the other hand, the eye is also drawn to point C on the curve, which corresponds to a set of size 29 with an FDP bound of 0.29. The $\hat{FDP}$ for this point is 0.12, so this set cannot be rejected by BH at level $q = 0.1$. However, both the $\hat{FD}$ and $\hat{FDP}$ curves suggest that set C has comparable purity to set A, even though it is much larger. If the extra 18 hypotheses looked promising to an investigator, she might prefer to go with set C. Meanwhile, note that the GS uniform bound provides much more conservative bounds over the relevant range. Finally, note that the choice $q = 0.1$ was decent, resulting in some discoveries. On the other hand, if the user had instead arbitrarily chosen $q = 0.05$, then BH would
have made no discoveries.

As demonstrated in this example, spotting can be more powerful than simultaneous inference while providing more flexibility than standard FDR control methods. Therefore, we suggest that simultaneous selective inference is a fruitful middle route between simultaneous and selective inference.

2.3. Summary of contributions. The main contribution of this paper is to prove uniform bounds of the form (6) for a variety of constructions of the path $\Pi$. It is important to choose the path to contain sets with low FDP, so that the menu presented to the user has some good options. While ordering hypotheses by p-values is a natural choice, power can be improved by leveraging any prior data containing information about which hypotheses are likely to be non-null. This insight has already been explored in the context of hypothesis testing with a priori ordering (Li and Barber, 2017; Lei and Fithian, 2016) or with ordering determined based on p-values as well as side information (Lei and Fithian, 2018; Lei, Ramdas and Fithian, 2017). We build on these works by borrowing their paths $\Pi$ and showing that multiplying their FDP estimates by small constants leads to uniform spotting bounds (6).

We provide spotting bounds in contexts beyond traditional multiple testing as well, including online testing and variable selection. In the online context, at each time point one hypothesis and its p-value arrive, and a decision to accept or reject must be made based on the information available at that time. Online FDR methods (Foster and Stine, 2008; Aharoni and Rosset, 2014; Javanmard and Montanari, 2017; Ramdas et al., 2018a) usually control the FDR marginally at each time point. Here, we provide high-probability FDP bounds simultaneously across all times for arbitrary online procedures, including all of the aforementioned ones and more.

In the variable selection context, interest lies in testing hypotheses of association between predictor variables and an outcome variable. The challenge, especially in high dimensions, is to obtain valid p-values for each variable. The knockoffs methodology (Barber and Candès, 2015; Candes et al., 2018) provides a solution to this issue by (1) ordering variables while creating independent “one-bit p-values” for each variable and then (2) applying an ordered FDR method to these p-values. Another methodology (G’Sell et al., 2016) leverages post-selection inference techniques to obtain valid p-values for sequential variable selection, and then applies an ordered FDR method to these p-values. The spotting bounds we derive for ordered testing procedures therefore automatically extend to the paths and p-values created by these two variable selection methodologies.
Aside from facilitating the prescriptive practice of spotting, our bounds also provide diagnostic information for FDR procedures in the form of high-probability FDP bounds for the rejection set. Indeed, since FDR procedures choose their rejection sets from a path, our bounds for FDP along that path can be applied. For instance, in the example from the previous section we got a high-probability upper bound of 0.36 for the BH rejection set. Furthermore, in certain cases our FDP bounds are a constant multiple of an existing procedure’s FDP estimate, i.e. $\hat{FDP}(\mathcal{R}_k) = c(\alpha) \cdot \hat{FDP}(\mathcal{R}_k)$. Since FDR procedures choose cutoffs based on the definition (11), our bound (6) also implies

$$\text{Pr}\{\text{FDP}(\mathcal{R}_k^*) \leq c(\alpha) \cdot q\} \geq 1 - \alpha,$$

i.e. these existing FDR procedures already guarantee control of the FDX at a constant multiple of the nominal FDR level $q$.

We prove our spotting bounds by developing a simple yet versatile proof technique to obtain tight non-asymptotic bounds for the probability that the stochastic process $|\mathcal{R}_k \cap \mathcal{H}_0|$ of false discoveries hits certain boundaries. We use martingale techniques that are rather different from the existing ones in the literature, as discussed in Sections 5 and 6.2. Thus, our work bridges the empirical process viewpoint and the martingale viewpoint on FDR procedures.

3. Main results. In this section, we present spotting bounds for various definitions of the path $\Pi$. We provide bounds for both the batch and online settings. In the batch setting, there is a finite number of hypotheses $H_1, \ldots, H_n$ for which the p-values are available all at once; in the online setting, where there is an infinite stream of hypotheses, which arrive one at a time and a decision must be made about each hypothesis as soon as its p-value arrives.

In each setting, we obtain spotting bounds via the following recipe. First, we consider a (regularized) estimate of the FDP of each set $\mathcal{R}_k$:

$$\hat{FDP}(\mathcal{R}_k) = a + \hat{V}(\mathcal{R}_k)/|\mathcal{R}_k|,$$

where $a \geq 0$ is an additive regularization and $\hat{V}(\mathcal{R}_k)$ is an estimate of $V(\mathcal{R}_k) \equiv |\mathcal{R}_k \cap \mathcal{H}_0|$. Often, the estimates $\hat{V}(\mathcal{R}_k)$ are borrowed from existing FDR procedures. While these existing procedures are defined using a fixed value of $a$, we consider using arbitrary regularizations $a > 0$. We then find
explicit constants \( c(\alpha) \) for which

\[
\Pr \left\{ \sup_{R \in \Pi} \frac{\text{FDP}(R)}{\text{FDP}(\hat{R})} \leq c(\alpha) \right\} \geq 1 - \alpha,
\]

We call these constants \textit{FDP multipliers}; note that they depend implicitly on \( \alpha, \hat{V}, \) and \( \pi \). Remarkably, these constants do not depend on \( n \). Based on this inequality, the spotting bound (6) immediately follows for

\[
\text{FDP}(\hat{R}) \equiv c(\alpha) \cdot \hat{\text{FDP}}(R_k).
\]

We now present several path constructions \( \pi \), corresponding estimates \( \hat{V} \), and the constants \( c(\alpha) \) for which the bound (14) holds. These settings are summarized in Table 1, and examples of the FDP multipliers \( c(\alpha) \) are given in Figure 2.

| \( \pi \)-[bound name] | p-val cutoffs | \( \hat{V}(\mathcal{R}_k) \) | FDR method |
|------------------------|--------------|----------------------------|-------------|
| sort                   | \( p_* = 1 \) | \( n \cdot p(k) \)        | BH          |
| preorder-acc           | \( p_* = 1 \) | \( \sum_{j \leq k} h(p_j) \) | Accumulation test |
| preorder-sel           | \( p_* \in (0, 1) \) | \( \sum_{j \leq k} \frac{p_*}{1 - \lambda_j} I(p_j > \lambda_j) \) | Selective and Adaptive SeqStep |
| interact-acc           | \( p_* = 1 \) | \( \sum_{j \leq k} h(p_{\pi(j)}) \) | STAR |
| interact-sel           | \( p_* \in (0, 1) \) | \( \sum_{j \leq k} \frac{p_*}{1 - \lambda_j} I(p_{\pi(j)} > \lambda_j) \) | AdapT |
| online-simple          | \( \alpha_j \in \mathcal{G}_{j-1} \) | \( \sum_{j \leq k} \frac{\alpha_j}{1 - \lambda_j} I(p_j > \lambda_j) \) | LORD, LORD++ |
| online-adaptive        | \( \alpha_j \in \mathcal{G}_{j-1} \) | \( \sum_{j \leq k} \frac{\alpha_j}{1 - \lambda_j} I(p_j > \lambda_j) \) | SAFFRON, alpha-investing |

Table 1

\textit{Overview of spotting bounds and FDR procedures inspiring them (\( h \) denotes an accumulation function).}

3.1. \textit{Spotting bounds in the batch setting.} Here, we have a fixed, finite set of hypotheses \( H_1, \ldots, H_n \) and a set of p-values \( p_1, \ldots, p_n \). To construct a path, consider first ordering the hypotheses in some way \( \sigma(1), \sigma(2), \ldots, \sigma(n) \), constructing \( \sigma \) to encourage non-nulls to appear near the beginning of the order. Then, define a p-value cutoff \( p_* \in (0, 1] \). We form a path \( \Pi \) by traversing the ordering and choosing hypotheses whose p-values passed the cutoff:

\[
\Pi \equiv (\mathcal{R}_0, \mathcal{R}_1, \ldots, \mathcal{R}_n) \text{ such that } \mathcal{R}_k \equiv \{ \sigma(j) : j \leq k, p_{\sigma(j)} \leq p_* \}.
\]

There are three ways of defining \( \pi \), each resulting in a different path:

1. \( \pi_{\text{sort}} \): \( \sigma \) is formed by sorting \( p \)-values as in (7), and taking \( p_* \equiv 1 \).
2. \( \pi_{\text{preorder}} \): \( \sigma \) is fixed ahead of time using prior knowledge.
3. \( \pi_{\text{interact}} \): \( \sigma \) is built on-the-fly using prior knowledge and \( p \)-values.

Next, we elaborate on these path constructions in the batch setting and present spotting bounds for each of them.
3.1.1. Spotting theorem for $\pi_{\text{sort}}$. Ordering hypotheses by p-value is the most common choice among multiple testing procedures and serves as the basis for the BH algorithm, the Benjamini-Liu stepdown procedure, and many others. It is the obvious choice when no side information is available. The following theorem presents FDP multipliers for this path construction.

**Theorem 1.** Let $\widehat{\Pi}_{\text{sort}}$ be defined via (13), with $a = 1$ and

$$\hat{V}_{\text{sort}}(\mathcal{R}_k) \equiv n \cdot p(k).$$

If the null p-values are independent and stochastically larger than uniform, i.e. $\Pr\{p_j \leq s\} \leq s$ for all $j \in \mathcal{H}_0$ and $s \in [0, 1]$, then the uniform bound (14) holds for $\Pi_{\text{sort}}$ for all $\alpha \in (0, 0.31]$, with

$$c_{\text{sort}}(\alpha) \equiv \frac{\log(\frac{1}{\alpha})}{\log\left(1 + \log\left(\frac{1}{\alpha}\right)\right)}.$$

Hence, spotting bound (6) holds with $\mathcal{FDP}(\mathcal{R}_k) \equiv c_{\text{sort}}(\alpha) \cdot \widehat{\Pi}_{\text{sort}}(\mathcal{R}_k)$.

**Remark 1.** In Theorem 1, we require that $\alpha \leq 0.31$. However, strong numerical evidence shows that the bound (14) is valid for $\Pi_{\text{sort}}$ with $c_{\text{sort}}(\alpha)$ for all $\alpha$. The restriction on $\alpha$ is an artifact of our proof and does not represent an intrinsic breaking point of the bound. Despite this limitation in our proof, the range $\alpha \leq 0.31$ comfortably includes any confidence level that would be used in practice (although the case $\alpha = 0.5$ might be of interest to bound the median of the distribution; for this we may rely on bound (46) in Section 6.3 below).

3.1.2. Spotting theorem for $\pi_{\text{preorder}}$. The pre-ordered setting applies when prior information (e.g. data from a similar experiment) sheds light on which hypotheses are more likely to be non-null, so a good ordering $\sigma$ is known in advance. Several FDR methodologies taking advantage of pre-specified orderings have been developed; G’Sell et al. (2016) and Li and Barber (2017) build paths using $p_\ast = 1$ while Barber and Candès (2015) and Lei and Fithian (2016) use $p_\ast (\in (0, 1)$.

For the case $p_\ast = 1$, we use a construction from the accumulation test of Li and Barber (2017): an accumulation function $h$ is a function $h : [0, 1] \to \mathbb{R}_+$ that is non-decreasing and integrates to 1. Then, we define

$$\hat{V}_{\text{preorder-acc}}(\mathcal{R}_k) \equiv \sum_{j=1}^{k} h(p_{\sigma(j)}).$$
Alternatively, for \( p^* \in (0, 1) \), we can follow Selective SeqStep (Barber and Candes, 2015) and Adaptive SeqStep (Lei and Fithian, 2016) to define

\[
\hat{V}_{\text{preorder-sel}}(\mathcal{R}_k) \equiv \sum_{j=1}^{k} \frac{p^*}{1 - \lambda} I(p_{\sigma(j)} > \lambda),
\]

where \( \lambda \geq p^* \). The following theorem presents FDP multipliers for \( \pi_{\text{preorder}} \) for both of the cases \( p^* = 1 \) and \( p^* \in (0, 1) \).

**Theorem 2.** Fix \( a > 0 \) and assume the null p-values are independent and stochastically larger than uniform.

1. Set \( p^* = 1 \), choose a (possibly unbounded) accumulation function \( h \), and define \( \hat{\text{FDP}}_{\text{preorder-acc}} \) via (13) and (19). Then, the uniform bound (14) holds for all \( \alpha \in (0, 1) \) with

\[
c_{\text{preorder-acc}}^h(\alpha) \equiv \frac{\log(\frac{1}{\alpha})}{a \log \left( \frac{\int_0^1 \alpha^{h(u)/a} du}{\alpha} \right)^{-1}}.
\]

Moreover, if \( \sup_{u \in [0,1]} h(u) \equiv B < \infty \), then we may instead use

\[
c_{\text{preorder-acc}}^B(\alpha) \equiv \frac{\log(\frac{1}{\alpha})}{a \log \left( 1 - \frac{1 - \alpha^B/a}{B} \right)^{-1}}.
\]

2. Set \( p^* \in (0, 1) \), fix \( \lambda \geq p^* \), and define \( \hat{\text{FDP}}_{\text{preorder-sel}} \) via (13) and (20). Then, uniform bound (14) holds for all \( \alpha \in (0, 1) \) with

\[
c_{\text{preorder-sel}}^B(\alpha) \equiv \frac{\log(\frac{1}{\alpha})}{a \log \left( 1 + \frac{1 - \alpha^B/a}{B} \right)^{-1}},
\]

where \( B \equiv \frac{p^*}{1 - \lambda} \). Hence the spotting bound (6) holds with \( \hat{\text{FDP}}(\mathcal{R}_k) \equiv c_{\text{preorder-}}(\alpha) \cdot \hat{\text{FDP}}_{\text{preorder-}}(\mathcal{R}_k) \).

3.1.3. Spotting theorem for \( \pi_{\text{interact}} \). In the interactive setting, hypotheses are ordered using a combination of side information \( x_j \) attached to each p-value and “masked” p-values. It is inspired by the recent methods AdaPT (Lei and Fithian, 2018) and STAR (Lei, Ramdas and Fithian, 2017), which use orthogonal parts of the information in the p-values to choose the path \( \Pi \) and where on the path to stop. Let \( g \) be a masking function, e.g.
Let $g(p) = \min(p, 1 - p)$ when $h(p) = 2I(p > 1/2)$. In this path construction, $\sigma(1)$ is chosen based on the information $\sigma(\{x_j, g(p_j)\}_{j \in [n]})$. Once $\sigma(1)$ is chosen, the corresponding p-value $p_{\sigma(1)}$ is unmasked, so the information $\sigma(\{x_j, g(p_j)\}_{j \in [n]}, p_{\sigma(1)})$ can be used to choose $\sigma(2)$. In general, we can choose $\sigma(k + 1)$ in any way based on the information

$$G_k \equiv \sigma(\{x_j, g(p_j)\}_{j \in [n]}, \{p_{\sigma(j)}\}_{j \leq k}).$$

Therefore, the ordering $\sigma$ may be built up interactively, with a human in the loop deciding the order based on $G_k$. We remark that this path construction differs slightly from that in AdaPT and STAR: we build up $\sigma$ from beginning to end, while these two methods proceed in the opposite direction. However, we do not expect this change to impact the quality of the constructed path.

The following theorem gives FDP multipliers for $\pi_{\text{interact}}$. Below, $h$ is always an accumulation function bounded by $B$ and $g$ is its corresponding masking function (see Lei, Ramdas and Fithian (2017)).

**Theorem 3.**

1. Set $p_\ast = 1$, let $\sigma$ be any ordering predictable with respect to the filtration (24), and define $\widehat{\text{FDP}}_{\text{interact-acc}} \equiv \text{FDP}_{\text{preorder-acc}}$. If the null p-values are independent of each other and of the non-null p-values, and the null p-values have non-decreasing densities, then uniform bound (14) holds for all $a > 0$ and all $\alpha \in (0, 1)$ with

$$c_{B_{\text{interact-acc}}}^B(\alpha) \equiv c_{B_{\text{preorder-acc}}}^B(\alpha).$$

2. Set $p_\ast \in (0, 1)$, fix $\lambda \geq p_\ast$, and choose $h(p) = I(p > \lambda)/(1 - \lambda)$ so that $B \equiv \frac{p_\ast}{1 - \lambda}$. Let $\sigma$ be any ordering predictable with respect to the filtration (24), and define $\widehat{\text{FDP}}_{\text{interact-sel}} \equiv \text{FDP}_{\text{preorder-sel}}$. If the null p-values are independent of each other and of the non-nulls, and the null p-values are mirror-conservative (see Lei and Fithian (2018)), then uniform bound (14) holds for all $\alpha \in (0, 1)$ with

$$c_{B_{\text{interact-sel}}}^B(\alpha) \equiv c_{B_{\text{preorder-sel}}}^B(\alpha).$$

Hence the spotting bound (6) holds with $\text{FDP}(R_k) \equiv c_{\text{interact-}}^\ast(\alpha) \cdot \text{FDP}_{\text{interact-}}^\ast(R_k)$.

These results bear obvious visual similarity to the previous section’s bounds, but are more subtle due to the data-dependent ordering $\sigma$.

### 3.2. Spotting theorem for any online algorithm

Now, we turn to spotting bounds for the online setting. In this setting, decisions about hypotheses must be made as they arrive one at a time in a stream. Moreover, the
order in which hypotheses arrive might or might not be the in the exper-
imen-ter’s control. Therefore, non-nulls might not necessarily occur early,
and further the rejection decision for the $H_k$ must be made without know-
ing the outcomes of future experiments. Hence, in general, online multiple
testing procedures must proceed differently from batch ones: online proce-
dures adaptively produce a sequence of levels $\alpha_j$ at which to test hypotheses.
Assuming for simplicity that $\sigma(j) = j$, these levels define the online path:

$$\Pi_{\text{online}} \equiv (R_1, R_2, \ldots R_n, \ldots)$$

where $R_k \equiv \{ j \leq k : p_j \leq \alpha_j \}$.

The levels $\alpha_j$ are chosen based on the outcomes of past experiments, i.e.

$$\alpha_{k+1} \in G_k \supseteq \sigma(I(p_j \leq \alpha_j); j \leq k).$$

The alpha-investing procedure of Foster and Stine (2008) and follow-up
works (Aharoni and Rosset, 2014; Javanmard and Montanari, 2017; Ram-
das et al., 2017) are built on the analogy of testing a hypothesis at level
$\alpha_j$ as spending wealth. One pays a price to test each hypothesis, and gets
rewarded for each rejected hypothesis. For each of these methods, the lev-
els $\alpha_j$ are adaptively constructed to ensure that the wealth always remains
non-negative. In this paper, we consider paths of the form (25) correspond-
ing to arbitrary sequences $\{\alpha_j\}$ satisfying requirement (26), including those
constructed by existing algorithms but any others as well.

Until recently, online FDR methods were formulated without reference
to any $FDP$. However, Ramdas et al. (2017) noted that LORD (Javanmard
and Montanari, 2017) implicitly bounds $\hat{FDP}(R_k)$ for $a = 0$ and

$$\hat{V}_{\text{online-simple}}(R_k) \equiv \sum_{j=1}^{k} \alpha_j.$$

They also used this fact to design a strictly more powerful algorithm called
LORD++. Moving beyond LORD++, Ramdas et al. (2018a) proposed an
adaptive algorithm called SAFFRON, which uses $a = 0$ and

$$\hat{V}_{\text{online-adaptive}}(R_k) \equiv \sum_{j=1}^{k} \frac{\alpha_j}{1 - \lambda_j} I(p_j > \lambda_j).$$

SAFFRON improves upon the LORD estimate by correcting for the pro-
portion of nulls, making it the online analog of the Storey-BH procedure
(Storey, Taylor and Siegmund, 2004). Like the levels $\alpha_j$, the constants $\lambda_j$
may also be chosen based on the outcomes of prior experiments.

The following theorem provides FDP multipliers corresponding to the
above two choices for $\hat{V}_{\text{online}}$. 
Theorem 4. Fix $a > 0$ and let $\alpha_1, \alpha_2, \ldots$ be any sequence of thresholds predictable with respect to filtration $G_k$, as in (26). Suppose the null p-values are stochastically larger than uniform conditional on the past:

$$\Pr\{p_k \leq s | G_{k-1}\} \leq s \quad \text{for each } k \in H_0 \text{ and each } s \in [0, 1].$$

1. If $\widehat{\text{FDP}}_{\text{online-simple}}$ is defined via (13) and (27), then uniform bound (14) holds for all $\alpha \in (0, 1)$ with

$$c_{\text{online-simple}}(\alpha) = \frac{\log(\frac{1}{\alpha})}{a \log \left(1 + \frac{\log(\frac{1}{\alpha})}{a}\right)}.$$  

2. Let $\lambda_j \geq \alpha_j$ for all $j$, $\{\lambda_j\}$ be predictable with respect to $G_k$, and $\sup_j \frac{\alpha_j}{\lambda_j} \equiv B < \infty$. If $\widehat{\text{FDP}}_{\text{online-adaptive}}$ is defined via (13) and (28), then uniform bound (14) holds for all $\alpha \in (0, 1)$ with

$$c^B_{\text{online-adaptive}}(\alpha) \equiv c^B_{\text{preorder-sel}}(\alpha).$$

Hence the spotting bound (6) holds with $\text{FDP}(R_k) \equiv c_{\text{online-}}^*(\alpha) \cdot \widehat{\text{FDP}}_{\text{online-}}^*(R_k)$.

3.3. Beyond multiple testing. All of the results presented here have been formulated in the multiple testing context, where we have p-values available for a set of hypotheses. However, these results also apply to model selection and variable selection contexts as well. In particular, G’Sell et al. (2016) proposed the ForwardStop accumulation function as a means to the end of model selection with FDR control. Using selective inference techniques, valid p-values may be obtained at each step of forward step-wise regression, and thus an accumulation test may be applied to select a model.

As another example, the knockoff filter by Barber and Candès (2015) was proposed for FDR control in the variable selection context. Their idea is to create a knockoff variable for each original variable, and then use these knockoffs as controls for the originals. Instead of p-values, the knockoff filter produces knockoff statistics $W_j$ for each variable $j$. However, the methodology is based on the fact that $\text{sign}(W_j)$ are independent fair coin flips for null $j$, in effect producing a set of “one-bit p-values”. Then, $c^B_{\text{preorder-sel}}$ with $p_*=0.5$ and $B=2$ may be applied to these one-bit p-values to select a set of variables with FDR control. Hence, our uniform bounds apply to the knockoff filter as well, with no additional assumptions. In particular, there is no need to specify a level $\alpha$ in advance to control FDR, and one may instead get post-hoc bounds uniformly over the knockoffs path.
3.4. Spotting bounds in expectation. Given the bound (14) on the quantiles of \( \sup_{R \in \Pi} \frac{FDP(R)}{FDP(\hat{R})} \), we may easily derive a bound on the expectation of this quantity. For \( \pi_{\text{sort}} \), define

\[
C_{\text{sort}} \equiv \int_0^{0.31} c_{\text{sort}}(\alpha) d\alpha + 0.69c_{\text{sort}}(0.31)
\]

and for other procedures, define

\[
C \equiv \int_0^1 c(\alpha) d\alpha.
\]

Then, we have the following corollary of the spotting theorems.

**Corollary 1.** For all proposed constructions of \( \Pi \) and \( \hat{FDP} \), we obtain the expected supremum ratio bound

\[
E \left[ \sup_{R \in \Pi} \frac{FDP(R)}{FDP(\hat{R})} \right] \leq C.
\]

The constants \( C \) are called FDR multipliers, and implicitly depend on \((\pi, a, \hat{V})\). For \( a = 1 \), we typically have \( C \leq 2 \). For example \( C_{\text{sort}} = 1.62, C_{\text{online-simple}} = 1.42, \) and \( C_{\text{B\emph{preorder-sel}}}^B = 1.92 \) for \( B = 2 \). See Figure 2 for more examples.

**Remark 2.** We only need to define \( C_{\text{sort}} \) in a special way due to the limitation of \( a \leq 0.31 \) in Theorem 1. If this restriction could be removed (see Remark 1), then we would obtain \( C_{\text{sort}} = 1.42 \).

A bound of the kind stated in Corollary 1 was first proved by Katsevich and Sabatti (2018) for \( \pi_{\text{preorder-sel}} \), with \( a = 1 \) and \( p_k = \lambda = 0.5 \), in the context of the multilayer knockoff filter, which is an extension of the p-filter (Barber and Ramdas, 2016; Ramdas et al., 2018b) to variable selection. The goal of that work was to prove FDR control for a predefined target level \( q \) with respect to multiple hypothesis groupings; the uniform bound was necessary because the more complicated form of \( k^* \) in that context precluded the use of standard martingale arguments.

Next, we inspect our bounds and probe their tightness numerically.

4. Inspecting the bounds. The goal of this section is to give concrete examples of the bounds we obtain in the previous section, and to show that these bounds are quite tight. To this end, we consider the following six choices for \((\pi, a, \hat{V})\), the first four corresponding to the batch setting and the last two to the online setting:

1. \( \pi_{\text{sort}}, a \equiv 1, \hat{V} \equiv \hat{V}_{\text{sort}} \).
2. $\pi_{\text{preorder}}, a \equiv 1, \hat{V} \equiv \hat{V}_{\text{preorder-acc}}$ with the SeqStep accumulation function $h(p) \equiv 2I(p > 0.5)$ (Barber and Candès, 2015).

3. $\pi_{\text{preorder}}, a \equiv 1, \hat{V} \equiv \hat{V}_{\text{preorder-sel}}$ with $p_* \equiv \lambda_* \equiv 0.5$.

4. $\pi_{\text{preorder}}, a \equiv 1, \hat{V} \equiv \hat{V}_{\text{preorder-sel}}$ with $p_* \equiv 0.05, \lambda_* \equiv 0.5$.

5. $\pi_{\text{online}}$ with $\alpha_k \equiv 0.05$ for all $k$, $a \equiv 1, \hat{V} \equiv \hat{V}_{\text{online-simple}}$.

6. $\pi_{\text{online}}$, with $\alpha_k \equiv 0.05$ for all $k$, $a \equiv 1, \hat{V} \equiv \hat{V}_{\text{online-adaptive}}$ with $\lambda_k \equiv 0.5$ for all $k$.

Figure 2 shows the FDP and FDR multipliers corresponding to each of these six settings. These multipliers, shown in red and cyan bars respectively, all correspond to the regularization $a = 1$. The procedures for pre-ordered paths (Accumulation tests, Selective SeqStep, Adaptive SeqStep) were originally proposed with positive regularization, and the multipliers corresponding to these original regularizations are shown using dashed bars. We observe some variability among the bounds across the six settings. Roughly, these differences can be understood as reflecting variability in $\hat{\text{FDP}}$ across these procedures. Certain FDP estimates are more stable than others; for example, the plot suggests that $\hat{\text{FDP}}_{\text{sort}}$ is more stable than $\hat{\text{FDP}}_{\text{preorder-sel}}$ with $p_* = 0.5$. This echoes the empirical observations that the BH method has a
fairly tight FDP histogram whereas the knockoffs procedure (which uses the estimate \( \hat{\text{FDP}}_{\text{preorder-sel}} \) with \( p_* = 0.5 \)) has more variability. This suggests that our FDP multipliers can provide insight into the variability of FDP for FDR procedures (see Section C in the supplement).

Next, we investigate the tightness of our bounds using numerical simulations. We simulated \( n = 500 \) independent test statistics \( X_j = \mu_j + \epsilon_j \), where \( \epsilon_j \sim N(0,1) \) and \( \mu_j = \mu I(j \in \mathcal{H}_1) \), for \( j = 1, \ldots, n \), and derived p-values \( p_j = 1 - \Phi(X_j) \). We chose a signal strength of \( \mu = 4 \); other signal strengths produced qualitatively similar figures. We simulated four sparsity settings, corresponding to \( |\mathcal{H}_1| = 0, 10, 25, 50 \). The locations of the signals were either chosen uniformly, or biased towards the beginning. For each setting, we generated 10,000 Monte Carlo realizations of \( \sup_k \frac{\text{FDP}(R_k)}{\text{FDP}(\hat{R}_k)} \).

Figure 3 shows the theoretical FDP multipliers (in black) and empirical realizations (in shades of blue) for the four batch settings above. We find that across the range of sparsity settings, the bounds are fairly tight. For \( \pi_{\text{sort}} \), the bounds get looser as the number of non-nulls increases, which reflects the fact that the \( \hat{\text{FDP}}_{\text{sort}} \) does not correct for the non-null proportion. For
relatively small non-null proportions (common in modern large-scale testing applications), this does not have a large effect. For the other three settings, the performance is not affected much by the sparsity level, because the definitions of FDP in those cases are relatively insensitive to non-nulls as long as their p-values are small enough. While our bounds \( c(\alpha) \) are smooth in all cases, we see that the Monte Carlo curves can be jagged, especially for second and third simulation settings. In these cases, this jaggedness reflects the discreteness of FDP.

![FDP Multipliers in the Online Setting](image)

**Figure 4.** (Online) The theoretically derived FDP bounds are generally tight, except for basic-online when signals are near the beginning. The online-adaptive estimate adapts to the non-null proportion and thus does not suffer from this issue.

Figure 4 shows the results of a similar simulation for the online setting, using choices 5 and 6 above. Unlike batch ordered testing, the signals for online testing do not necessarily occur near the beginning, so in addition we considered the situation when signals are randomly located. Like for \( \pi_{sort} \), we find that the bounds for basic-online get looser as the sparsity fraction increases. While for randomly located signals the difference is not very large,
for signals near the beginning we see that the basic-online bound becomes quite conservative. This is because the “local” non-null fraction near the beginning is large even if the overall non-null fraction is not, resulting in much looser bounds. On the other hand, we find that the online-adaptive bounds are fairly tight across sparsity levels and signal locations.

Next, we provide a glimpse of the proof of our spotting theorems.

5. A key lemma. In this section, we present a key exponential tail inequality lemma (Lemma 1) that underlies the proofs of Theorems 2, 3, and 4. The proof of Theorem 1 requires a more involved proof technique, which we defer to the supplementary materials, where we also show how Theorems 2, 3, and 4 follow from Lemma 1 below. We use a martingale-based proof technique that is distinct from the technique used to prove FDR control; see Section 6.2 for a comparison.

Lemma 1. Consider a (potentially infinite) set of hypotheses \( H_1, H_2, \ldots \), an ordering \( \sigma(1), \sigma(2), \ldots \), and a set of cutoffs \( \alpha_1, \alpha_2, \ldots \). Let

\[
\mathcal{R}_k \equiv \{ j \leq k : p_{\sigma(j)} \leq \alpha_j \} \quad \text{and} \quad \widehat{\text{FDP}}(\mathcal{R}_k) \equiv \frac{a + \sum_{j \leq k} h_j(p_{\sigma(j)})}{|\mathcal{R}_k|},
\]

where \( \{h_j\}_{j \geq 1} \) are functions on \([0, 1]\). Suppose there exists a filtration

\[
\mathcal{F}_k \supseteq \sigma(\mathcal{H}_0, \{\sigma(j)\}_{j \leq k}, \{h_j(p_{\sigma(j)}), I(p_j \leq \alpha_j)\}_{j \leq k, \sigma(j) \in \mathcal{H}_0}).
\]

such that for all \( \sigma(k) \in \mathcal{H}_0 \), we have

\[
\text{Pr}\{p_{\sigma(k)} \leq \alpha_k \mid \mathcal{F}_{k-1}\} \leq \alpha_k \quad \text{and} \quad \mathbb{E}[h_k(p_{\sigma(k)}) \mid \mathcal{F}_{k-1}] \geq \alpha_k,
\]

almost surely. Then, for each \( x > 1 \) and \( a > 0 \),

\[
\text{Pr}\left\{ \sup_{k} \frac{\text{FDP}(\mathcal{R}_k)}{\text{FDP}(\mathcal{R}_k)} \geq x \right\} \leq \exp(-a \theta_x x),
\]

where \( \theta_x \) is defined in the following four cases:

1. If \( h_k = h \) for some accumulation function \( h \), \( \alpha_k = 1 \), \( \sigma(k) \) is pre-specified (i.e. nonrandom), and \( p_{\sigma(k)} \perp \mathcal{F}_{k-1} \) for all \( \sigma(k) \in \mathcal{H}_0 \), then \( \theta_x \) is the unique positive root of the equation

\[
\int_0^1 \exp(-\theta x h(u)) du = \exp(-\theta).
\]
2. If \( h_k = h \) for some accumulation function \( h \) bounded by \( B \) and \( \alpha_k = 1 \), then \( \theta_x \) is the unique positive root of the equation
\[
\exp(-\theta) + \frac{1 - \exp(-\theta x B)}{B} = 1.
\]

3. If \( h_k(p) = 0 \) for all \( p \leq \alpha_k \), and \( h_k(p) \leq B \) for all \( k, p \), then \( \theta_x \) is the unique positive root of the equation
\[
\exp(\theta) - \frac{1 - \exp(-\theta x B)}{B} = 1.
\]

4. If \( h_k(p_k) = \alpha_k \), then \( \theta_x \) is the unique positive root of the equation
\[
e^\theta = 1 + \theta x.
\]

**Proof.** Fix any arbitrary \( x > 1 \) and \( \theta > 0 \). We first restrict our attention to only the nulls as follows:

\[
\Pr \left\{ \sup_k \frac{\text{FDP}(R_k)}{\text{FDP}(R_k)} \geq x \right\} = \Pr \left\{ \sup_k \frac{V(R_k)}{a + V(R_k)} \geq x \right\}
\]

\[
= \Pr \left\{ \sum_{j=1}^{k} I(p_{\sigma(j)} \leq \alpha_j) I(\sigma(j) \in \mathcal{H}_0) \geq ax + x \sum_{j=1}^{k} h_j(p_{\sigma(j)}), \text{ for some } k \right\}
\]

\[
\leq \Pr \left\{ \sum_{j=1}^{k} I(p_{\sigma(j)} \leq \alpha_j) I(\sigma(j) \in \mathcal{H}_0) \geq ax + x \sum_{j=1}^{k} h_j(p_{\sigma(j)}) I(\sigma(j) \in \mathcal{H}_0), \text{ for some } k \right\}.
\]

Now, we may rearrange terms and employ the Chernoff exponentiation trick, to conclude that:

\[
\Pr \left\{ \sup_k \frac{\text{FDP}(R_k)}{\text{FDP}(R_k)} \geq x \right\}
\]

\[
= \Pr \left\{ \sup_k \exp \left( \theta \left( \sum_{j=1}^{k} [I(p_{\sigma(j)} \leq \alpha_j) - xh_j(p_{\sigma(j)})] I(\sigma(j) \in \mathcal{H}_0) \right) \right) \geq \exp(a \theta x) \right\}
\]

\[
\equiv \Pr \left\{ \sup_k Z_k \geq \exp(a \theta x) \right\}.
\]

We claim that if \( \theta = \theta_x \), then \( Z_k \) is a supermartingale with respect to \( \mathcal{F}_k \). If this is the case, then the conclusion of the lemma would follow from the Ville (1939) maximal inequality for positive supermartingales:

\[
\Pr \left\{ \sup_k Z_k \geq \exp(a \theta x) \right\} \leq \exp(-a \theta x) \mathbb{E}[Z_0] = \exp(-a \theta x),
\]
as desired. Hence the rest of this proof will focus on showing the super-
martingale property of $Z_k$. Note first of all that $Z_k$ is adapted to $F_k$ by
assumption (33). Hence, it suffices to show that

$$
\mathbb{E} \left[ \frac{Z_k}{Z_{k-1}} \bigg| F_{k-1} \right] = \mathbb{E} \left[ \exp \left\{ \theta (I(p_{\sigma(k)}) \leq \alpha_k) - xh_k(p_{\sigma(k)}) \right\} \bigg| F_{k-1} \right] \leq 1.
$$

Clearly, this inequality holds for any $k$ such that $\sigma(k) \not\in \mathcal{H}_0$. For $k$ such that $\sigma(k) \in \mathcal{H}_0$, we find that

$$
\mathbb{E} \left[ \exp \left\{ \theta (I(p_{\sigma(k)}) \leq \alpha_k) - xh_k(p_{\sigma(k)}) \right\} \bigg| F_{k-1} \right] 
= \mathbb{E} \left[ I(p_{\sigma(k)} \leq \alpha_k) \exp \left\{ \theta (1 - xh_k(p_{\sigma(k)}) \right\} \bigg| F_{k-1} \right] 
+ \mathbb{E} \left[ I(p_{\sigma(k)} > \alpha_k) \exp \left\{ -\theta xh_k(p_{\sigma(k)}) \right\} \bigg| F_{k-1} \right].
$$

(41)

To show that the above quantity is at most one, we consider the four cases
defined in the statement of the lemma.

**Case 1.** Since $\alpha_k = 1$, the second term of equation (41) equals zero. Since $h_k = h$, $\sigma(k)$ is fixed, and $p_{\sigma(k)} \perp F_{k-1}$, the first term simplifies to

$$
\mathbb{E} \left[ \exp \left\{ \theta x(1 - xh(p_{\sigma(k)}) \right\} \bigg| F_{k-1} \right] = \mathbb{E} \left[ \exp \left\{ \theta x(1 - xh(p_{\sigma(k)}) \right\} \bigg| F_{k-1} \right] 
\leq \exp(\theta x)\mathbb{E}_{U \sim U[0,1]} \left[ \exp(-\theta xh(U)) \right] 
= 1,
$$

The inequality holds because $p_{\sigma(k)}$ is superuniformly distributed by assumption and $u \mapsto \exp(-\theta xh(u))$ is a nonincreasing function (since $h$ is nondecreasing by definition), and the last step holds because $\theta x$ satisfies equation (36) by definition.

**Case 2.** Again, the second term of equation (41) equals zero because $\alpha_k = 1$. We may bound the first term as:

$$
\mathbb{E} \left[ \exp \left\{ \theta x(1 - xh(p_{\sigma(k)}) \right\} \bigg| F_{k-1} \right] \leq \exp(\theta x)\mathbb{E} \left[ 1 - \frac{1 - \exp(-\theta xB)}{B}h(p_{\sigma(k)}) \bigg| F_{k-1} \right] 
\leq \exp(\theta x) \left( 1 - \frac{1 - \exp(-\theta xB)}{B} \right) 
= 1.
$$

In the first line, we used the fact that $h_k(p_{\sigma(k)}) = h(p_{\sigma(k)}) \leq B$, and we bounded the convex function $z \mapsto \exp(-\theta xz)$ on $[0, B]$ with the line $z \mapsto 1 - \frac{1 - \exp(-\theta xB)}{B} z$. In the second step, we used the assumption $\mathbb{E} \left[ h(p_{\sigma(k)}) \bigg| F_{k-1} \right] \geq \alpha_k = 1$, and in the third line we used the definition of $\theta x$. 
Case 3. Because $h_k(p)I(p \leq \alpha_k) = 0$, the first term of equation (41) simplifies to
\[
\mathbb{E} \left[ I(p_{\sigma(k)} \leq \alpha_k) \exp \{ \theta_x (1 - x h_k(p_{\sigma(k)}) \} \mid F_{k-1} \right] = \exp(\theta_x) \Pr\{ p_{\sigma(k)} \leq \alpha_k \mid F_{k-1} \}.
\]

To bound the second term, we write
\[
\mathbb{E} \left[ I(p_{\sigma(k)} > \alpha_k) \exp \{ -\theta_x x h_k(p_{\sigma(k)}) \} \mid F_{k-1} \right]
\leq \mathbb{E} \left[ I(p_{\sigma(k)} > \alpha_k) \left( 1 - \frac{1 - \exp(-\theta_x x B)}{B} h_k(p_{\sigma(k)}) \right) \mid F_{k-1} \right]
\]
\[
= \Pr\{ p_{\sigma(k)} > \alpha_k \mid F_{k-1} \} - \frac{1 - \exp(-\theta_x x B)}{B} \mathbb{E} \left[ h_k(p_{\sigma(k)}) I(p_{\sigma(k)} > \alpha_k) \mid F_{k-1} \right]
\]
\[
= \Pr\{ p_{\sigma(k)} > \alpha_k \mid F_{k-1} \} - \frac{1 - \exp(-\theta_x x B)}{B} \Pr\{ p_{\sigma(k)} > \alpha_k \mid F_{k-1} \}
\]
\[
\leq \Pr\{ p_{\sigma(k)} > \alpha_k \mid F_{k-1} \} - \frac{1 - \exp(-\theta_x x B)}{B} \alpha_k.
\]

The inequality in the second line follows from the same convexity argument as in Case 2, the fourth line is a consequence of the fact that $h_k(p)I(p \leq \alpha_k) = 0$, and the last line follows from $\mathbb{E} \left[ h_k(p_{\sigma(k)}) \mid F_{k-1} \right] \geq \alpha_k$.

Combining the results of the previous two equations, we obtain that
\[
\mathbb{E} \left[ I(p_{\sigma(k)} \leq \alpha_k) \exp \{ \theta_x (1 - x h_k(p_{\sigma(k)}) \} \mid F_{k-1} \right] + \mathbb{E} \left[ I(p_{\sigma(k)} > \alpha_k) \exp \{ -\theta_x x h_k(p_{\sigma(k)}) \} \mid F_{k-1} \right]
\leq \exp(\theta_x) \Pr\{ p_{\sigma(k)} \leq \alpha_k \mid F_{k-1} \} + \Pr\{ p_{\sigma(k)} > \alpha_k \mid F_{k-1} \} - \frac{1 - \exp(-\theta_x x B)}{B} \alpha_k
\]
\[
= (\exp(\theta_x) - 1) \Pr\{ p_{\sigma(k)} \leq \alpha_k \mid F_{k-1} \} + 1 - \frac{1 - \exp(-\theta_x x B)}{B} \alpha_k
\]
\[
\leq (\exp(\theta_x) - 1) \alpha_k + 1 - \frac{1 - \exp(-\theta_x x B)}{B} \alpha_k
\]
\[
= \alpha_k \left( \exp(\theta_x) - 1 - \frac{1 - \exp(-\theta_x x B)}{B} \right) + 1
\]
\[
= 1.
\]

The inequality in the fourth line follows from the first part of assumption (34), and the last equality follows from the definition of $\theta_x$.

Case 4: Since $h_k(p) = \alpha_k$, equation (41) simplifies to:
\[
\exp(\theta_x (1 - x \alpha_k)) \Pr\{ p_{\sigma(k)} \leq \alpha_k \mid F_{k-1} \} + \exp(-\theta_x x \alpha_k) \Pr\{ p_{\sigma(k)} > \alpha_k \mid F_{k-1} \}
\]
\[
= \exp(-\theta_x x \alpha_k) ((\exp(\theta_x) - 1) \Pr\{ p_{\sigma(k)} \leq \alpha_k \mid F_{k-1} \} + 1)
\]
\[
\leq \exp(-\theta_x x \alpha_k) ((\exp(\theta_x) - 1) \alpha_k + 1).
\]
Noting that $\theta_x$ satisfies (39), we see that the above expression can be bounded by one:

$$\exp(-\theta_x x \alpha_k) (\theta_x x \alpha_k + 1) \leq 1,$$

as desired, where the inequality follows because the function $z \mapsto e^{-z}(z + 1)$ is decreasing and takes the value 1 at $z = 0$. \hfill \Box

See Section A.2 in the supplementary materials for proofs of Theorems 2, 3, and 4 based on Lemma 1. See Section A.1 for the proof of Theorem 1.

6. Comparisons to work on FDR control. The paths and spotting bounds we construct are tied to existing FDR control algorithms. In this section, we explore the relationships between our results and those already existing in the FDR literature.

6.1. Comparing the roles of $\hat{\text{FDP}}$. We start by recalling the definition (13) of $\hat{\text{FDP}}$. Batch FDR algorithms use this estimate of FDP to automatically choose the rejection set $R^* \in \Pi$, which is done via (11). On the other hand, we use $\hat{\text{FDP}}$ as a building block for our confidence envelopes $\overline{\text{FDP}}$ (recall definition (15)), which the user may then inspect to choose $R^*$. It is important to remark here that while our spotting bounds are inspired by existing FDR algorithms, they are not intrinsically tied to the use of those procedures in any way. Indeed, we often employ the path $\Pi$ of known FDR or FDX procedures, but not their stopping criterion or choice of final rejected set.

Each FDR algorithm comes with a “built-in” choice of regularization $a$. For example, the BH algorithm uses no regularization (i.e. $a = 0$), while accumulation tests (Li and Barber, 2017) use $a = \sup_{u \in [0,1]} h(u)$. The built-in regularizations are chosen to ensure FDR control (see below). On the other hand, we consider arbitrary regularizations $a > 0$, with different regularizations leading to different FDP multipliers $c(\alpha)$ and therefore different confidence envelopes. Different regularization parameters lead to envelopes that are tight in different places; see the discussion in Section 7 and Section C in the supplementary materials.

6.2. Comparing proof techniques. For each existing batch FDR algorithm, FDR control is established using the following martingale argument. First, the ratio $\frac{\text{FDP}(R_k)}{\hat{\text{FDP}}(R_k)} = \frac{V(\overline{R}_k)}{a + V(\overline{R}_k)}$ is upper-bounded by a stochastic process $L_k$, such that $L_k$ is a supermartingale with respect to a backwards filtration.
Furthermore, it is shown that $\mathbb{E} [L_n] \leq 1$. The choice of regularization $a$ is usually made to ensure the existence of such an $L_k$. Using the fact that $k^*$ picked using rule (11) is a stopping time with respect to $\Omega_k$, we obtain $\text{FDR} = \mathbb{E} [\text{FDP}(\mathcal{R}_{k^*})] \leq q$ in a single line using the optional stopping theorem:

$$\mathbb{E} [\text{FDP}(\mathcal{R}_{k^*})] \leq \mathbb{E} \left[ \frac{\text{FDP}(\mathcal{R}_{k^*})}{\hat{\text{FDP}}(\mathcal{R}_{k^*})} \right] \leq \mathbb{E} [L_{k^*}] \leq 1.$$ (42)

This technique was first used by Storey, Taylor and Siegmund (2004) for the BH procedure, but remarkably, the other batch procedures mentioned in this paper like knockoffs, AdaPT, STAR, ordered tests and others, all implicitly use the same argument (though it was not expressed as succinctly as above), each with different $L_k, \Omega_k$.

Note that while we also rely on a martingale argument to prove our spotting bounds (recall Section 5), the martingales we construct are fundamentally different: they are exponential and employ forward filtrations instead of backwards ones.

6.3. Connections between spotting bounds and existing FDR results. By comparing our uniform FDP bound (14) with the FDR proof (42), we see that both hinge on bounding the ratio $\frac{\text{FDP}(\mathcal{R})}{\hat{\text{FDP}}(\mathcal{R})}$.

FDR control is established via

$$\mathbb{E} \left[ \frac{\text{FDP}(\mathcal{R}^*)}{\hat{\text{FDP}}(\mathcal{R}^*)} \right] \leq 1;$$ (43)

i.e. on average, $\hat{\text{FDP}}$ does not underestimate FDP for the rejection set $\mathcal{R}^*$. On the other hand, Corollary 1 states that

$$\mathbb{E} \left[ \sup_{\mathcal{R} \in \Pi} \frac{\text{FDP}(\mathcal{R})}{\hat{\text{FDP}}(\mathcal{R})} \right] \leq C,$$ (44)

where $C$ is a small constant (less than 2 in most cases). Comparing (43) and (44), we see that moving from an expectation bound only on $\mathcal{R}^*$ to a simultaneous bound over all $\mathcal{R} \in \Pi$ costs us only a small multiplicative factor, which is usually smaller than 2.

All the spotting theorems (including bound (44)) require some form of independence among the p-values. Aside from BH, the FDR procedure corresponding to each of our spotting bounds also requires independence to show (43). Furthermore, our assumptions for each of these theorems are
identical to or weaker than the ones needed to prove FDR control. For Theorem 1, we only need to make assumptions on the distribution \((p_j)_{j \in H_0}\), so unlike existing proofs of FDR control for BH, we do not make any assumptions on the dependence of the nulls on the non-nulls. In Theorem 2, we assume that the nulls are independent and stochastically larger than uniform, whereas for the original FDR control results (Barber and Candès, 2015; Li and Barber, 2017) it was also required that nulls be independent of non-nulls. In Theorems 3 and 4, our assumptions are identical to those in the original works.

For FDR algorithms whose built-in regularization is positive (those relying on pre-ordered and interactively constructed paths, including the knockoffs procedure for variable selection), bound (14) states that FDP is not much larger than \(\hat{\text{FDP}}\) over the entire path of FDR algorithms. Focusing on the set \(R^*\), this implies that

\[
\Pr\{\text{FDP}(R_k^*) \leq c(\alpha) \cdot q\} \geq 1 - \alpha,
\]

i.e. these FDR procedures also control FDX at level \(c(\alpha) \cdot q\). The dashed bars in Figure 2 are FDP multipliers \(c(\alpha)\) corresponding to original regularizations \(a\). To our knowledge, these are the first nontrivial finite-sample FDX bounds for FDR procedures (though crude bounds based on Markov’s inequality were proposed by Lehmann and Romano (2005)).

Finally, note that upper confidence bands of the form (14) can also be derived from the supermartingales \((L_k, \Omega_k)\) used to prove FDR control for batch procedures. Indeed, using Ville’s maximal inequality again, we find

\[
\Pr\left\{\sup_{0 \leq k \leq n} \frac{\text{FDP}(R_k)}{\text{FDP}(R_k)} \geq x\right\} \leq \Pr\left\{\sup_{0 \leq k \leq n} L_k \geq x\right\} \leq \frac{1}{x} \mathbb{E}[L_n] \leq \frac{1}{x}.
\]

In other words, for each batch procedure we consider, the upper confidence band (14) holds with original regularization and \(c(\alpha) = \alpha^{-1}\). Versions of this bound have been considered before in the case of BH, e.g. by Robbins (1954) and Goeman et al. (2016). The above inequality immediately implies that each batch FDR procedure (when applied in the standard way at predefined level \(q\)) implicitly controls the FDX at level \(\frac{2}{\alpha}\) with probability \(1 - \alpha\). The above bound also implies that for all considered batch procedures, we have

\[
\text{Median} \left[\sup_{R \in \Pi} \frac{\text{FDP}(R)}{\text{FDP}(R)}\right] \leq 2.
\]

However, note that the constants \(c(\alpha) = \alpha^{-1}\) grow quickly as \(\alpha\) decays. On the other hand, the constants we provide scale logarithmically, rather than linearly, in \(\alpha^{-1}\).
7. Comparisons to prior work on simultaneous inference. As discussed in Section 2, our results are connected to existing work on simultaneous upper confidence bounds on FDP. Broadly, some procedures (van der Laan, Dudoit and Pollard, 2004; Genovese and Wasserman, 2006; Goeman and Solari, 2011) construct high-probability bounds FDP simultaneously for all subsets \( \mathcal{R} \subseteq [n] \), as in (2), while others (Genovese and Wasserman, 2004; Meinshausen, 2006) bound FDP for the sets \( \mathcal{R}_t \equiv \{ j : p_j \leq t \} \):

\[
\Pr\{ \text{FDP}(\mathcal{R}_t) \leq \text{FDP}(\mathcal{R}_t) \text{ for all } t \in [0,1] \} \geq 1 - \alpha.
\]

The latter kind of FDP bounds can be extended to any other sets, as pointed out implicitly by Genovese and Wasserman (2006) and Goeman and Solari (2011), and explicitly by more recent work (Blanchard, Neuvial and Roquain, 2017). In particular, this implies that our uniform bounds on FDP(\( \mathcal{R}_k \)) can also be extended to uniform bounds on all subsets.

We leave the exhaustive comparison of our spotting bounds with existing simultaneous bounds for future work. However, we pause here to make some remarks on this topic. First of all, we expect that in certain cases, simultaneous selective bounds can be less conservative than simultaneous bounds over all subsets. While it is intuitive that less simultaneity should imply less conservatism, it was pointed out by a referee that this might depend on how the sets for which guarantees are given are selected. For example, if they are selected by p-value order (as in BH), then we might need to pay for this selection in the form of more conservative bounds, making it unclear whether spotting bounds can do better than fully simultaneous bounds. On the other hand, we expect that in settings where the selection of the path relies on prior or side information, the simultaneous selective inference approach can be much less conservative than simultaneous inference.

We begin probing these issues here with two simple simulations in the context of \( \pi_{\text{sort}} \) and \( \pi_{\text{preorder-sel}} \) (with \( p_* = \lambda = 0.1 \)). In both cases, we compare the average shape of the FDP upper bounds obtained from spotting and from GS’s simultaneous bounds (at \( \alpha = 0.1 \)). The simulation setup for \( \pi_{\text{sort}} \) is the same as the one from the introduction. For \( \pi_{\text{preorder-sel}} \), the setup is the same except we randomly scatter 25 signals of size 3 between positions 10 and 60. Figure 5 shows in magenta and blue the FDP upper bounds of spotting and GS, respectively, averaged over 100 repetitions. The black curves are the average true FDP. We see that spotting generally outperforms GS, but the difference is much bigger in the case of \( \pi_{\text{preorder-sel}} \), where spotting can take advantage of the informative ordering.

In the batch setting, the existing bounds that are most directly comparable with ours are those of the form (47). Meinshausen and Rice (2006)
propose two explicit, finite-sample bounds of the form $\overline{\text{FDP}}(R_t) \equiv V(t)$:

$$V_{\text{Robbins}}(t) \equiv \frac{1}{\alpha} nt; \quad V_{\text{DKW}}(t) \equiv \sqrt{\frac{n}{2} \log \frac{1}{\alpha}} + nt.$$ 

These bounds derive from those found by Robbins (1954) and Dvoretzky, Kiefer and Wolfowitz (1956), respectively. Compare these to our bound, which is

$$V_{\text{sort}}(t) \equiv c_{\text{sort}}(\alpha) + c_{\text{sort}}(\alpha) \cdot nt.$$ 

Note that $\mathbb{E} [\|R_t \cap H_0\|] \leq nt$, and that each definition of $V$ inflates this quantity in order to obtain the simultaneous high-probability bound (47). The Robbins bound is fully multiplicative and the DKW bound is fully additive, while the spotting bound contains additive and multiplicative elements. The additive elements have more effect for small $t$ than multiplicative elements, so the DKW bound is the tightest when $t$ is large, the Robbins bound is the tightest when $t$ is small, and the spotting bound is the tightest in an intermediate range. We see this in Figure 6, which compares the three bounds for $n = 500$ and $\alpha = 0.05$. The dotted vertical lines indicate the Bonferroni level and the nominal level, respectively. The interval between these two
levels is the most interesting for multiple testing, and the spotting bound is the tightest over most of this range (in particular, it is tighter than the Robbins bound as long as $V_{\text{Robbins}}(t) \geq 2.4$). In fact, the spotting bound is not too far from the pointwise $1 - \alpha$ quantile of $V(t)$, which is plotted for reference in black in the left panel. The right panel shows the p-values at which the supremum in equation (14) is achieved. We see that the majority of the time (about 62%), the supremum for the spotting bound is attained in the interesting range.

We saw in the above comparison that multiple confidence envelopes can be constructed for the same path, each tight in a certain region of the path. Note that our spotting theorems also provide multiple confidence envelopes for the same path. For example, different accumulation functions $h$ can be used to define $\tilde{V}_{\text{preorder-acc}}$. For all of our bounds (except for the $\pi_{\text{sort}}$ bound), we may also vary the regularization parameter $\alpha$. There is a nontrivial trade-off involved in selecting these “tuning parameters”: decreasing $\tilde{FDP}$ has the effect of increasing $c(\alpha)$; see Section C in the supplementary materials. We leave for future work the investigation of these trade-offs and the design of the tightest confidence envelopes for a given part of the path.

There has also been work on providing confidence envelopes such that the bound (47) holds asymptotically as $n \to \infty$, e.g. by Storey, Taylor and

**Fig 6.** Comparing spotting bounds to two other explicit finite-sample bounds for $\pi_{\text{sort}}$, with $n = 500$ and $\alpha = 0.05$. Vertical dotted lines indicate Bonferroni level $\alpha/n$ and nominal level $\alpha$, between which is the “interesting” range of cutoffs. The left panel shows the three spotting bounds and the right panel shows histograms of the p-values where the supremum in (14) is achieved. The spotting bound is tightest across most of the interesting range.
In the online setting, the closest result is that of Javanmard and Montanari (2017) (JM). JM consider a truncated version of generalized alpha-investing rules that satisfy a uniform FDX bound like $\Pr \{ \sup_k FDP_k \geq \gamma \} \leq \alpha$. Their result is similar in spirit to our result in Theorem 4 about $\hat{FDP}_{\text{online-simple}}$, but there are some subtle differences. Their results, like most other FDX bounds, are pre hoc, meaning that given a $\gamma, \alpha \in (0, 1)$, their procedure produces a sequence of rejections satisfying the desired FDX guarantee. Our guarantees are post hoc, meaning that they would apply to any sequence of rejections produced by any online algorithm, that may or may not have been designed for FDR or FDP control.

Finally, we are not currently aware of confidence envelopes that explicitly leverage side information in the form of covariates, a priori hypothesis orderings, and so on. From this point of view, the envelopes $FDP(\mathcal{R}_k) \equiv c(\alpha) \cdot \hat{FDP}(\mathcal{R}_k)$ we derived for all procedures except BH represent the first uniform FDX bounds in structured settings.

8. Conclusion. We have shown in this paper that under independence, for a variety of procedures in the literature, the estimate $\hat{FDP}$ (with regularization added if necessary) actually bounds the unknown FDP not just on average for the rejected set, but also up to a small constant factor with high probability over the entire path of rejected sets proposed by each procedure.

This nontrivial and somewhat surprising result yields uniform upper bounds on FDP across a variety of paths, including the standard BH path as well as paths that leverage side information to better order hypotheses. These results pave the way for “simultaneous selective inference.” Instead of picking a single rejected set out of $2^n$, we can use the same machinery to efficiently carve out a path of $n$ rejected sets based on structural constraints or prior knowledge, provide a uniform upper confidence band for the unknown FDP, and allow the user to choose one or more rejection sets in hindsight, providing simultaneous guarantees over all such rejection sets.

Our bounds also provide new guarantees for old procedures. In particular, they show that the achieved FDP of ordered and interactive FDR procedures (which also includes variable selection procedures like knockoffs) is bounded by a constant factor $c(\alpha)$ times the FDR target level $q$ with probability at least $1 - \alpha$. For all procedures (designed for FDR control or otherwise) choosing their rejection set from a path we consider, our bounds also provide diagnostic information in the form of a high-probability bound on the FDP.

Note that all of the results in this paper have assumed independence of
p-values in one form or another. Many of the procedures considered here also only have guarantees under independence, though BH is a notable exception. Aside from online testing applications, independent p-values are hard to come by in practice, so more robust guarantees are necessary. BH is known to control FDR under the PRDS criterion (Benjamini and Yekutieli, 2001), a form of positive dependence that contains no information about the strength of the dependence. However, it is known that while the mean of FDP might not change much as dependence increases, the variance of the FDP will increase (Owen, 2005; Efron, 2010). Hence, high-probability bounds on FDP under dependence are likely to use criteria other than PRDS to capture this dependence. As a first step in this direction, we empirically investigate in Section D of the supplementary materials how the bounds change under local correlation. We find that most of our bounds are fairly robust to negative correlations and moderate positive correlations, with some being more sensitive to correlation than others. We leave the pursuit of simultaneous selective inference in dependent settings for future work.

As pointed out to us by a referee, our bounds may also be used to construct new tests of the global null. Moreover, following Meinshausen and Rice (2006), our uniform bounds can also be used to estimate the null proportion among a set of hypotheses. Exploring these consequences of our spotting bounds is an interesting direction for future work.

Finally, the proof technique we developed in this paper is versatile enough to cover a large portion of the currently available FDR procedures. Like Genovese and Wasserman (2004), we employ a stochastic process approach to analyze the FDP. However, while GW’s bounds are asymptotic, we have used martingale arguments instead to obtain tight, non-asymptotic bounds. Perhaps these proof techniques may be extended further to apply to other multiple testing scenarios as well.

9. Acknowledgements. E.K. would like to thank Chiara Sabatti for her generous and valuable feedback on this work and on the manuscript itself, as well as David Siegmund, Emmanuel Candes, Anya Katsevich, and Michael Sklar for helpful discussions. A.R. acknowledges fruitful conversations with Ohad Feldheim, Jim Pitman and Jon Wellner. Both authors are also grateful for the insightful comments of the referees and associate editor.

SUPPLEMENTARY MATERIAL

Supplement:
(doi: COMPLETED BY THE TYPESETER; .pdf). Proofs of all theorems and supplementary discussion.
References.

Aharoni, E. and Rosset, S. (2014). Generalized α-investing: definitions, optimality results and application to public databases. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 76 771–794.

Anderson, G. D., Barnard, R. W., Richards, K. C., Vamanamurthy, M. K. and Vuorinen, M. (1995). Inequalities for zero-balanced hypergeometric functions. *Transactions of the American Mathematical Society* 1713–1723.

Barber, R. F. and Candès, E. J. (2015). Controlling the false discovery rate via knockoffs. *The Annals of Statistics* 43 2055–2085.

Barber, R. F. and Ramdas, A. (2016). The p-filter: multilayer false discovery rate control for grouped hypotheses. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*.

Benjamini, Y. and Hochberg, Y. (1995). Controlling the false discovery rate: a practical and powerful approach to multiple testing. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 57 289–300. MR1325392 (96d:62143)

Benjamini, Y. and Liu, W. (1999). A step-down multiple hypotheses testing procedure that controls the false discovery rate under independence. *Journal of Statistical Planning and Inference* 82 163–170.

Benjamini, Y. and Yekutieli, D. (2001). The control of the false discovery rate in multiple testing under dependency. *The Annals of Statistics* 29 1165–1188.

Blanchard, G., Neuvial, P. and Roquain, E. (2017). Post hoc inference via joint family-wise error rate control. *arXiv preprint arXiv:1703.02307*.

Candes, E., Fan, Y., Janson, L. and Lv, J. (2018). Panning for gold: ‘model-X’ knockoffs for high dimensional controlled variable selection. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 80 551–577.

Dobriban, E. (2018). Flexible Multiple Testing with the FACT Algorithm. *arXiv preprint arXiv:1806.10163*.

Dvoretzky, A., Kiefer, J. and Wolfowitz, J. (1956). Asymptotic minimax character of the sample distribution function and of the classical multinomial estimator. *The Annals of Mathematical Statistics* 642–669.

Efron, B. (2010). *Large-scale inference*. Institute of Mathematical Statistics (IMS) Monographs 1. Cambridge University Press, Cambridge Empirical Bayes methods for estimation, testing, and prediction.

Finner, H. and Roters, M. (2001). On the false discovery rate and expected type I errors. *Biometrical Journal* 43 985–1005.

Foster, D. P. and Stine, R. A. (2008). α-investing; a procedure for sequential control of expected false discoveries. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 70 429–444.

Genovese, C. and Wasserman, L. (2004). A stochastic process approach to false discovery control. *The Annals of Statistics* 1035–1061.

Genovese, C. R. and Wasserman, L. (2006). Exceedance control of the false discovery proportion. *Journal of the American Statistical Association* 101 1408–1417.

Goeman, J. and Solari, A. (2011). Multiple testing for exploratory research. *Statistical Science* 584–597.

Goeman, J., Meijer, R., Koots, T. and Solari, A. (2016). Simultaneous Control of All False Discovery Proportions in Large-Scale Multiple Hypothesis Testing. *arXiv preprint arXiv:1611.06739*.

G’Sell, M. G., Wager, S., Chouldechova, A. and Tibshirani, R. (2016). Sequential selection procedures and false discovery rate control. *Journal of the Royal Statistical
Javanmard, A. and Montanari, A. (2017). Online Rules for Control of False Discovery Rate and False Discovery Exceedance. The Annals of Statistics.

Katsevich, E. and Sabatti, C. (2018). Multilayer Knockoff Filter: Controlled variable selection at multiple resolutions. Annals of Applied Statistics (accepted).

Lehmann, E. L. and Romano, J. (2005). Generalizations of the familywise error rate. The Annals of Statistics 1138–1154.

Lei, L. and Fithian, W. (2016). Power of ordered hypothesis testing. In International Conference on Machine Learning 2924–2932.

Lei, L. and Fithian, W. (2018). AdaPT: an interactive procedure for multiple testing with side information. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 80 649–679.

Lei, L., Ramdas, A. and Fithian, W. (2017). STAR: A general interactive framework for FDR control under structural constraints. arXiv preprint arXiv:1710.02776.

Li, A. and Barber, R. F. (2016). Accumulation tests for FDR control in ordered hypothesis testing. Journal of the American Statistical Association 1–13.

Meijer, R., Krebs, R., Solari, A. and Goeman, J. (2017). A shortcut for Hommel’s procedure in linearthmic time. arXiv preprint arXiv:1710.08273.

Meinshausen, N. (2006). False discovery control for multiple tests of association under general dependence. Scandinavian Journal of Statistics 33 227–237.

Meinshausen, N. and Rice, J. (2006). Estimating the proportion of false null hypotheses among a large number of independently tested hypotheses. The Annals of Statistics 34 373–393.

Owen, A. B. (2005). Variance of the number of false discoveries. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 67 411–426.

Ramdas, A., Yang, F., Wainwright, M. J. and Jordan, M. I. (2017). Online control of the false discovery rate with decaying memory. In Advances In Neural Information Processing Systems.

Ramdas, A., Zrnic, T., Wainwright, M. and Jordan, M. (2018a). SAFFRON: an Adaptive Algorithm for Online Control of the False Discovery Rate. In Proceedings of the 35th International Conference on Machine Learning 4286–4294.

Ramdas, A., Barber, R. F., Wainwright, M. and Jordan, M. (2018b). A unified treatment of multiple testing with prior knowledge using the p-filter. Annals of Statistics (accepted).

Robbins, H. (1954). A one-sided confidence interval for an unknown distribution function. In Annals of Mathematical Statistics 25 409–409.

Storey, J. (2002). A direct approach to false discovery rates. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 64 479–498. MR1924302 (2003h:62029)

Storey, J., Taylor, J. and Siegmund, D. (2004). Strong control, conservative point estimation and simultaneous conservative consistency of false discovery rates: a unified approach. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 66 187–205.

Troendle, J. F. (2000). Stepwise normal theory multiple test procedures controlling the false discovery rate. Journal of Statistical Planning and Inference 84 139–158.

Van der Laan, M. J., Dudoit, S. and Pollard, K. S. (2004). Multiple testing. Part III. Procedures for control of the generalized family-wise error rate and proportion of false positives.

Ville, J. (1939). Étude Critique de la Notion de Collectif. Gauthier-Villars, Paris.
APPENDIX A: PROOFS OF THE FOUR SPOTTING THEOREMS

The method we employ to obtain all our FDP multipliers is to investigate the properties of the stochastic process $\text{FDP}(R_k)$. Below, we prove the optional spotting theorems; the proof of Corollary 1 will follow from the fact that the expectation of a random variable is the integral of its quantile function. We start with the $\pi_{\text{sort}}$ path construction, for which we must proceed differently since the hypotheses are ordered according to the p-values, while for all other settings, the hypothesis order is either pre-specified or is in some sense “orthogonal” to FDP.

A.1. Proof of Theorem 1.

Proof. Let $V_t \equiv \sum_{j \in H_0} I(p_j \leq t)$, and let $V'_t$ be distributed as the unscaled empirical process of $n$ independent uniformly distributed random variables. Then, for any fixed $x > 1$ and $a = 1$ we have

$$\Pr \left\{ \sup_k \frac{\text{FDP}(R_k)}{\text{FDP}(R_k)} \geq x \right\} = \Pr \left\{ \sup_{t \in [0,1]} \frac{V_t}{1 + nt} \geq x \right\}$$

$$\leq \Pr \left\{ \sup_{t \in [0,1]} \frac{V'_t}{1 + nt} \geq x \right\}$$

$$= \Pr \{ V'_t \geq x + xnt, \text{ for some } t \in [0,1] \} .$$

The second inequality holds because $V'_t$ is stochastically larger than $V_t$ because $n \geq |H_0|$ and because the p-values are assumed to be stochastically larger than uniform. Hence, the quantity of interest is the probability that the stochastic process $V'_t$ hits the linear boundary $x + xnt$. This event is illustrated in Figure 7.

However, it is somewhat difficult to obtain non-asymptotic bounds for probabilities that empirical processes like $V'_t$ hit certain boundaries. Instead, we claim that for $x \geq 1.5$, replacing $V'_t$ with a rate $n$ Poisson process $N_t$ only further increases the hitting probability:

$$\Pr \{ V'_t \geq x + xnt, \text{ for some } t \in [0,1] \} \leq \Pr \{ N_t \geq x + xnt, \text{ for some } t \in [0,1] \} .$$

See Appendix B for the proof of this lemma. To understand why the lemma holds, note that $V'_t \overset{d}{=} N_t|N_1 = n$; i.e. the distribution of the empirical
process is the same as that of the Poisson process, conditioned on observing exactly $n$ events at time $t = 1$. Hence, Lemma 2 states that for sufficiently large $x$, a Poisson process is less likely to hit the line $t \mapsto t + xnt$ if we know that it is equal to its mean at time $t = 1$. This makes intuitive sense because the process needs to be far above its mean to hit this line for large $x$, which is less likely to happen if it must be equal to its mean at time $t = 1$.

Now, we may use the martingale properties of Poisson processes to bound the probability a Poisson process hits a linear boundary:

**Lemma 3 (Katsevich and Sabatti (2018)).** If $N_t$ is a rate $n$ Poisson process, then for any $x > 1$, we have

$$\Pr\{N_t \geq x + xnt \text{ for some } t \in [0, 1]\} \leq \exp(-x\theta_x),$$

where $\theta_x$ is the unique positive root of the equation (39) in the main text.

To complete the derivation of the FDP multiplier for $\pi_{\text{sort}}$, suppose we choose $x$ such that $\alpha = \exp(-x\theta_x)$. Then, plugging this choice of $x$ into the definition of $\theta_x$ implies that

$$x = \frac{-\log \alpha}{\theta_x} = \frac{-\log \alpha}{\log(1 + \theta_x x)} = \frac{-\log \alpha}{\log(1 - \log \alpha)} = c_{\pi_{\text{sort}}} (\alpha),$$

where $c_{\pi_{\text{sort}}} (\alpha)$ is defined in the main text.
which proves the bound (18). Hence, statement (14) holds for all $\alpha$ corresponding to $x \geq 1.5$, which translates to holding for all $\alpha \leq 0.31$, since $c_{\pi_{\text{sort}}}(0.31) = 1.5$.

A.2. Proofs of Theorems 2, 3, and 4. Here, we derive Theorems 2, 3, and 4 as corollaries of Lemma 1 presented in the main text.

Proof of Theorem 2. In this case, the ordering $\sigma$ is pre-specified, so we may assume without loss of generality that $\sigma(j) = j$. First we note that the filtration

$$\mathcal{F}_k = \sigma(H_0, \{p_j\}_{j \leq k, j \in H_0})$$

satisfies the required condition (33). Next, we consider $\pi_{\text{preorder-acc}}$ and $\pi_{\text{preorder-sel}}$ separately.

1. $\pi_{\text{preorder-acc}}$: For any $k \in H_0$, since $\alpha_k = 1$, the first part of the requirement (34) is trivially satisfied. To show the second part, we use the independence assumption in Theorem 2 and the assumed superuniformity of null p-values to derive

$$\mathbb{E}[h_k(p_k) | \mathcal{F}_{k-1}] = \mathbb{E}[h(p_k)] \geq \mathbb{E}_{U \sim U[0,1]}[h(U)] = \int_0^1 h(u)du = 1 = \alpha_k.$$ 

The inequality follows because $p_k$ is superuniform and $h$ is nondecreasing. Hence, the assumptions of Lemma 1, case 1 are satisfied, so the bound (35) holds with $\theta_x$ satisfying equation (36). In order to prove the bound (21), we simply note that for any $\alpha \in (0,1)$, we may choose $x$ such that $\exp(-a\theta_x x) = \alpha$, from which it follows that

$$x = \frac{-\log \alpha}{a \theta_x} = \frac{\log \alpha}{a \log \int_0^1 \exp(-\theta_x x h(u))du} = \frac{\log \alpha}{a \log \int_0^1 \alpha^{h(u)/a}du} = c_{\text{acc}}^h(\alpha),$$

as desired.

If the accumulation function is bounded by $B$, then the assumptions of Lemma 1, case 2 are also satisfied, so the bound (35) holds with $\theta_x$ satisfying equation (37). In order to prove the bound (22), we note that for any $\alpha \in (0,1)$, we may choose $x$ such that $\exp(-a\theta_x x) = \alpha$, from which it follows that

$$x = \frac{-\log \alpha}{a \theta_x} = \frac{\log \alpha}{a \log \left(1 - \frac{1 - \exp(-\theta_x x B)}{B}\right)} = \frac{\log \alpha}{a \log \left(1 - \frac{1 - \alpha B/a}{B}\right)} = c_{\text{acc}}^B(\alpha),$$

as desired.
2. \( \pi_{\text{preorder-sel}} \): We claim that the assumptions of Lemma 1 are satisfied with \( F_k \) defined as in equation (51). Indeed, fix \( k \in \mathcal{H}_0 \). Then, the assumed superuniformity of null p-values implies that
\[
\Pr\{p_k \leq \alpha_k \mid F_{k-1}\} = \Pr\{p_k \leq p_*\} \leq p_* = \alpha_k
\]
and
\[
\mathbb{E}\left[h_k(p_k) \mid F_{k-1}\right] = \mathbb{E}\left[\frac{p_*}{1-\lambda} I(p > \lambda)\right] \geq p_* = \alpha_k.
\]
Hence, by case 3 of Lemma 1, it follows that (35) holds for \( \theta_x \) satisfying (38). For fixed \( \alpha \in (0, 1) \), define \( x \) such that \( \exp(-a\theta_x x) = \alpha \). Then,
\[
x = \frac{-\log \alpha}{a \theta_x} = \frac{-\log \alpha}{a \log \left(1 + \frac{1-\exp(-\theta_x x B)}{B}\right)} = \frac{-\log \alpha}{a \log \left(1 + \frac{1-\alpha^{B/a}}{B}\right)} = c_{AS}(\alpha),
\]
which proves the bound (23).

\[\square\]

**Proof of Theorem 3.** This proof is similar to that of Theorem 2, except the filtrations must be somewhat more complicated to accommodate the interactivity of \( \pi_{\text{interact-acc}} \) and \( \pi_{\text{interact-sel}} \). For both of these path constructions, define the filtration
\[
F_k = \sigma(\mathcal{H}_0, \{x_j, g(p_j)\}_{j \in [n]}, \{p_{\sigma(j)}\}_{j \leq k}).
\]
Since \( \sigma \) is predictable with respect to the filtration \( G_k \) (24) by the definition of \( \pi_{\text{interact-acc}} \) and \( F_k \supset G_k \), it follows that \( \sigma \) is also predictable with respect to \( F_k \). Hence, requirement (33) holds for \( F_k \) as defined above. Now, let \( \sigma(k) \in \mathcal{H}_0 \).

For \( \pi_{\text{interact-sel}} \), the first part of condition (34) holds because
\[
\Pr\{p_{\sigma(k)} \leq \alpha_k \mid F_{k-1}\} = \mathbb{E}\left[\Pr\{p_{\sigma(k)} \leq p_* \mid g(p_{\sigma(k)}), \sigma(k)\} \mid \sigma(k)\right]
\leq \Pr_{U \sim U[0,1]}\{U \leq p_* \mid g(U)\}
= p_*
= \alpha_k.
\]

The first equality follows from the independence assumption on the p-values, the first inequality follows from the predictability of \( \sigma(k) \) and from the assumption that the null p-values have increasing densities (see the proof of
Proposition 1 in Lei, Ramdas and Fithian (2017)). Similarly,

$$E[h_k(p_{\sigma(k)}) \mid \mathcal{F}_{k-1}] = E\left[E\left[\frac{p_*}{1-p_*} I(p_{\sigma(k)}>p_*) \mid g(p_{\sigma(k)}), \sigma(k)\right] \mid \sigma(k)\right]$$

$$\geq \frac{p_*}{1-p_*} Pr_{U \sim U[0,1]}\{U > p_* \mid g(U)\} = p_* = \alpha_k.$$

For $\pi_{\text{interact-acc}}$, the first part of condition (34) is trivially satisfied. To derive the second part, we write

$$E[h_k(p_{\sigma(k)}) \mid \mathcal{F}_{k-1}] = E\left[E\left[h_k(p_{\sigma(k)}) \mid g(p_{\sigma(k)}), \sigma(k)\right] \mid \sigma(k)\right]$$

$$\geq E_{U \sim [0,1]}[h(U)g(U)] = 1 = \alpha_k.$$

The justification for this derivation is similar to that for $\pi_{\text{interact-sel}}$, noting in addition that $E_{U \sim [0,1]}[h(U)g(U)] = 1$ by construction.

Having established that the assumptions of Lemma 1 are satisfied for $\pi_{\text{interact-sel}}$ and $\pi_{\text{interact-acc}}$, the rest of the proof follows exactly as in the proof of Theorem 2.

**Proof of Theorem 4.** Let $G_k$ be the filtration defined in the statement of Theorem 4. Define

$$(52) \quad \mathcal{F}_k \equiv \sigma(G_k, \mathcal{H}_0).$$

Then, assumption (33) clearly holds for $\pi_{\text{online-simple}}$ and $\pi_{\text{online-adaptive}}$ by (26). The first part of (34) holds for both online procedures considered by assumption (29). For $\pi_{\text{online-simple}}$, the second part holds because $h_k(p_k) = \alpha_k$. For $\pi_{\text{online-adaptive}}$, the second part holds because for $k \in \mathcal{H}_0$,

$$E[h_k(p_k) \mid \mathcal{F}_{k-1}] = E\left[\frac{\alpha_k}{1-\lambda_k} I(p_k > \lambda_k) \mid \mathcal{F}_{k-1}\right] \geq \alpha_k,$$

where the last step follows from the predictability of $\alpha_k$ and $\lambda_k$ and the assumption (29).

Hence, $\pi_{\text{online-simple}}$ and $\pi_{\text{online-adaptive}}$ satisfy the assumptions of Lemma 1. The remainder of the proof corresponds exactly to analogous parts of the earlier proofs described for $\pi_{\text{sort}}$ and $\pi_{\text{preorder-sel}}$, respectively. \qed
APPENDIX B: FROM EMPIRICAL TO POISSON PROCESSES

Proof of Lemma 2. Let \( \{N_t\}_{t \geq 0} \) be a Poisson process with rate \( n \). It suffices to show that for \( x \geq 1.5 \),

\[
\mathbb{P} \left[ \sup_{t \in [0,1]} \frac{N_t}{1 + nt} \geq x \, \middle| \, N_1 = n \right] \leq \mathbb{P} \left[ \sup_{t \in [0,1]} \frac{N_t}{1 + nt} \geq x \right].
\]

Let us define

\[
\tau = \inf \left\{ t : \frac{N_t}{1 + nt} \geq x \right\}.
\]

We claim that it suffices to show that for \( x \geq 1.5 \),

\[
\mathbb{P}[N_1 = n | \tau] \leq \mathbb{P}[N_1 = n] \quad \text{for all } \tau \geq 0.
\]

Indeed, it would then follow that

\[
\mathbb{P} \left[ \sup_{t \in [0,1]} \frac{N_t}{1 + nt} \geq x \, \middle| \, N_1 = n \right] = \mathbb{P} \left[ \tau \leq 1 \middle| N_1 = n \right]
\]

\[
= \frac{\mathbb{P}[\tau \leq 1] \mathbb{P}[N_1 = n | \tau \leq 1]}{\mathbb{P}[N_1 = n]}
\]

\[
\leq \mathbb{P}[\tau \leq 1]
\]

\[
= \mathbb{P} \left[ \sup_{t \in [0,1]} \frac{N_t}{1 + nt} \geq x \right].
\]

Note that for a given \( x \), \( x(1 + nt) > n \) for \( t > \frac{1}{x} - \frac{1}{n} \). Hence, statement (54) is trivial for \( \tau > \frac{1}{x} - \frac{1}{n} \), so we need only consider

\[
\tau \leq \frac{1}{x} - \frac{1}{n}.
\]

Define

\[
f(\lambda, y) = e^{-\lambda} \frac{\lambda^y}{\Gamma(y + 1)}.
\]

This function \( f : [0, \infty) \rightarrow \mathbb{R} \) is equal to the probability mass function of the Poisson with parameter \( \lambda \) when \( y \in \{0, 1, 2, \ldots\} \). We have

\[
\mathbb{P}[N_1 = n | \tau] = \mathbb{P}[N_1 = n | N_\tau = [x(1 + n\tau)]
\]

\[
= \mathbb{P}[N_{1-\tau} = n - [x(1 + n\tau)]]
\]

\[
= f(n(1 - \tau), n - [x(1 + n\tau)])
\]

\[
\leq f(n(1 - \tau), n - x(1 + n\tau))
\]

\[
\equiv g(\tau, x).
\]
The inequality follows by Lemma 5 because \( n - x(1 + n\tau) \leq n(1 - \tau) - x \leq n(1 - \tau) - 1.5 \). Define

\[
(58) \quad h(\tau, x) = \log g(\tau, x) = \log \left( \exp(-n(1 - \tau)) \frac{(n(1 - \tau))^{n-x(1+n\tau)}}{\Gamma(1+n-x(1+n\tau))} \right) \\
= -n(1 - \tau) + (n - x(1 + n\tau)) \log(n(1 - \tau)) - \log \Gamma(1 + n - x(1 + n\tau)).
\]

Note that

\[
(59) \quad \frac{\partial}{\partial \tau} h(\tau, x) \\
= n - xn \log(n(1 - \tau)) - \frac{n - x(1 + n\tau)}{1 - \tau} + xn\psi(1 + n - x(1 + n\tau)) \\
\leq n - xn \log(n(1 - \tau)) - \frac{n - x(1 + n\tau)}{1 - \tau} + xn \left( \log(1.5 + n - x(1 + n\tau)) - \frac{1}{1.5 + n - x(1 + n\tau)} \right) \\
\equiv r(\tau, x).
\]

The inequality follows by Lemma 4.

To prove the inequality (54), it suffices to show that

(a) \( g(0, x) \leq \mathbb{P}[N_1 = n] \) for all \( x \geq 1.5 \);
(b) \( r(\tau, 1.5) \leq 0 \) for each \( \tau \leq \frac{1}{1.5} - \frac{1}{n} \);
(c) \( \frac{\partial}{\partial \tau} r(\tau, 1.5) \leq 0 \) for each \( \tau \leq \frac{1}{1.5} - \frac{1}{n} \);
(d) \( r(\tau, x) \) is concave in \( x \) for each \( \tau \).

Indeed, note that (c) and (d) imply that for each \( \tau \leq \frac{1}{1.5} - \frac{1}{n} \), \( r(\tau, x) \) is a decreasing function of \( x \) for \( x \geq 1.5 \). Hence, for each \( x \geq 1.5 \) and each \( \tau \), we have \( r(\tau, x) \leq r(\tau, 1.5) \leq 0 \), where the last inequality follows from (b). Hence, by inequality (59), \( \frac{\partial h}{\partial \tau}(\tau, x) \leq r(\tau, x) \leq 0 \) for each \( x \geq 1.5 \). This means that \( h(\tau, x) \) is decreasing in \( \tau \) for each \( x \geq 1.5 \), so \( g(\tau, x) \) is decreasing in \( \tau \) for each \( x \geq 1.5 \), from which it follows that \( g(\tau, x) \leq g(0, x) \leq \mathbb{P}[N_1 = n] \), where the last inequality follows by (a).

Proof of (a). We have

\[
g(0, x) = f(n, n - x) \leq f(n, n - 1) = f(n, n) = \mathbb{P}[N_1 = n].
\]

where the inequality follows by Lemma 5 and the equality \( f(n - 1, n) = f(n, n) \) holds because

\[
\frac{f(n, n - 1)}{f(n, n)} = \frac{n^{n-1}}{\Gamma(n)} \frac{\Gamma(n)}{\Gamma(n+1)} = \frac{\Gamma(n + 1)}{n\Gamma(n)} = 1.
\]
Proof of (b). We have

\[ r(\tau, 1.5) = n - 1.5n \log(n(1 - \tau)) - \frac{n - 1.5(1 + n\tau)}{1 - \tau} \]
\[ + 1.5n \left( \log(1.5 + n - 1.5(1 + n\tau)) - \frac{1}{1.5 + n - 1.5(1 + n\tau)} \right) \]
\[ = n - 1.5n \log(n(1 - \tau)) - \frac{n - n\tau - 1.5 - 0.5n\tau}{1 - \tau} + 1.5n \left( \log(n(1 - 1.5\tau)) - \frac{1}{n(1 - 1.5\tau)} \right) \]
\[ = 1.5n \log \left( \frac{1 - 1.5\tau}{1 - \tau} \right) + \frac{1.5 + 0.5n\tau}{1 - \tau} - \frac{1.5}{1 - 1.5\tau} \]
\[ = n \left( 1.5 \log \left( \frac{1 - 1.5\tau}{1 - \tau} \right) + \frac{0.5\tau}{1 - \tau} \right) + 1.5 \left( \frac{1}{1 - \tau} - \frac{1}{1 - 1.5\tau} \right) \]
\[ \leq n \left( 1.5 \log \left( \frac{1 - 1.5\tau}{1 - \tau} \right) + \frac{0.5\tau}{1 - \tau} \right) \]
\[ = n \left( -1.5 \frac{0.5\tau}{1 - \tau} + \frac{0.5\tau}{1 - \tau} \right) \]
\[ = -n \frac{0.25\tau}{1 - \tau} \]
\[ \leq 0. \]

Proof of (c). We have

\[ \frac{\partial r}{\partial x}(\tau, x) = -n \log(n(1 - \tau)) + \frac{1 + n\tau}{1 - \tau} + n \log(1.5 + n - x(1 + n\tau)) \]
\[ - \frac{(1 + n\tau)xn}{1.5 + n - x(1 + n\tau)} - n \frac{1.5 + n - x(1 + n\tau) + x(1 + n\tau)}{(1.5 + n - x(1 + n\tau))^2} \]
\[ = -n \log(n(1 - \tau)) + \frac{1 + n\tau}{1 - \tau} + n \log(1.5 + n - x(1 + n\tau)) \]
\[ - \frac{(1 + n\tau)xn}{1.5 + n - x(1 + n\tau)} - n \frac{1.5 + n}{(1.5 + n - x(1 + n\tau))^2}. \]
Plugging in $x = 1.5$, we have

$$
\frac{\partial r}{\partial x}(\tau, 1.5) = -n \log(n(1 - \tau)) + \frac{1 + n\tau}{1 - \tau} + \log(n(1 - 1.5\tau)) - \frac{1.5(1 + n\tau)n}{n(1 - 1.5\tau)} \leq \frac{1.5 + n}{n(1 - 1.5\tau)}
$$

$$
\leq n \left( \log \left( \frac{1 - 1.5\tau}{1 - \tau} \right) + \frac{\tau}{1 - \tau} - \frac{1.5\tau}{1 - 1.5\tau} \right) \leq n \left( \log \left( \frac{1 - 1.5\tau}{1 - \tau} \right) + \frac{\tau}{1 - \tau} - \frac{1.5\tau}{1 - 1.5\tau} \right)
$$

$$
\leq n \left( \frac{-0.5\tau}{1 - \tau} + \frac{\tau}{1 - \tau} - \frac{1.5\tau}{1 - 1.5\tau} \right).
$$

$$
= n \left( \frac{0.5\tau}{1 - \tau} - \frac{1.5\tau}{1 - 1.5\tau} \right).
$$

$$
\leq n \left( \frac{\tau(0.75\tau - 1)}{1 - \tau(1 - 1.5\tau)} \right).
$$

$$
\leq 0,
$$

where the last inequality follows because $\tau \leq \frac{1}{1.5} - \frac{1}{n} \leq 4/3$.

Proof of (d). Modulo terms linear in $x$ and the scaling factor $n$, $r(\tau, x)$ is equal to

$$
x \log (1.5 + n - x(1 + n\tau)) - \frac{x}{1.5 + n - x(1 + n\tau)}.
$$

We claim that the first term is concave in $x$ and the second term is convex, from which it will follow that their difference is concave. By linear transformations, the concavity of the first term will follow from the concavity of $x \log(1 - x)$, which follows because its first derivative $\log(1 - x) - \frac{x}{1 - x}$ is decreasing in $x$. Again by linear transformations, the convexity of the second term will follow from the convexity of $\frac{x}{1-x} = -1 + \frac{1}{1-x}$ on $x < 1$, which is clear.

**Lemma 4.** Let $\psi(x) = \Gamma'(x)/\Gamma(x)$ be the digamma function. Then, $\psi$ is increasing, and for $x \geq 1$,

$$
\psi(x) \leq \log(x) - \frac{1}{2x} \leq \log(x + 0.5) - \frac{1}{x + 0.5} \leq \log x.
$$

**Proof.** The fact that $\psi$ is increasing is well-known. The first inequality follows directly from Theorem 3.1 of Anderson et al. (1995). To prove the
second inequality, write
\[ \log(x + 0.5) - \log(x) = \log\left(1 + \frac{0.5}{x}\right) \geq \frac{0.5}{x} - \frac{1}{2} \left(\frac{0.5}{x}\right)^2, \]
and the conclusion follows because
\[ \frac{0.5}{x} - \frac{1}{2} \left(\frac{0.5}{x}\right)^2 \geq \frac{1}{x + 0.5} - \frac{1}{2x} \iff \frac{1}{2x} - \frac{1}{8x^2} \geq \frac{x - 0.5}{2x(x + 0.5)} \iff x \geq 1/6. \]
To prove the third inequality, write
\[ \log(x + 0.5) - \log(x) = \log\left(1 + \frac{0.5}{x}\right) \leq \frac{0.5}{x}, \]
and the conclusion follows because
\[ \frac{0.5}{x} \leq \frac{1}{x + 0.5} \iff x \geq 0.5. \]

**Lemma 5.** Let $f$ be as defined in equation (56). Then,
\[ \frac{\partial}{\partial y} f(\lambda, y) \geq 0 \quad \text{for all } y \leq \lambda - 1. \]

**Proof.** To prove this, it suffices to show that for $y \leq \lambda - 1$,
\[ 0 \leq \frac{\partial}{\partial y} \log f(\lambda, y) = \frac{\partial}{\partial y} (-\lambda + y \log \lambda - \log \Gamma(y + 1)) = \log \lambda - \psi(y + 1). \]
Indeed, by Lemma 4, for $y \leq \lambda - 1$ we have $\psi(y + 1) \leq \psi(\lambda) \leq \log \lambda$. 

**APPENDIX C: TRADE-OFFS BETWEEN FDP ESTIMATES AND MULTIPLIERS**

Note that by varying the “tuning parameters” for each of our bounds (like the regularization $a$ or the accumulation function $h$ for $\pi_{\text{preorder-acc}}$), we get multiple confidence envelopes for the same path $\Pi$. Getting the “best” confidence envelope
\[ \FDP(R) = c(\alpha) \cdot \tilde{\FDP}(R) \]
for a given path is nontrivial, since decreasing $\tilde{\FDP}$ tends to increase $c(\alpha)$. Moreover, Figure 6 in the main text suggests that confidence envelopes that are tighter in one part of the path tend to be looser in another. In this section,
we illustrate these trade-offs in the context of choosing an accumulation function for $\pi_{\text{preorder-acc}}$.

We consider the SeqStep, HingeExp, and ForwardStop accumulation functions (see Barber and Candès (2015); Li and Barber (2017); G’Sell et al. (2016), respectively), truncated if necessary to be bounded by $B = 2$. The left panel of Figure 8 depicts these three accumulation functions and the right panel shows the corresponding FDP multipliers. We observe that steeper accumulation functions have larger FDP multipliers. This reflects the fact that for a uniform random variable $U$, $h(U)$ is more variable if $h$ is steeper, since this random variable has more mass at its extremes. This translates to an increase in the variance of $\hat{FDP}$ and therefore an increase in the multiplier $c(\alpha)$.

![Figure 8](image)

**Fig 8.** Three accumulation functions and the corresponding FDP multipliers. Note that the steeper the accumulation function, the larger the FDP multiplier.

Now, we compare the confidence envelopes resulting from these three accumulation functions via numerical simulation. We use the same simulation setup as in Section 4 of the main text, with 50 non-nulls, except we decrease the signal amplitude to $\mu = 2.5$. The left panel of Figure 9 depicts the $\hat{FDP}$ curves, averaged over 10,000 simulations. For comparison, the black curve is the average true FDP. We find that the steeper accumulation functions have less upwardly-biased FDP estimates. Therefore, smaller FDP estimates correspond to larger $c(\alpha)$. We see this trade-off in action in the right panel of Figure 9, which shows the confidence envelopes for FDP, with the black curve representing the pointwise $1 - \alpha$ quantiles for the true FDP as a reference. We find that SeqStep has the smallest $\hat{FDP}$ but the largest $c(\alpha)$, and
as a result leads to the worst FDP bound. ForwardStop and HingeExp both give better bounds than SeqStep, with HingeExp being a little better over the most interesting range of \( k \), around 25-50. Hence, HingeExp strikes the best balance between power and FDP variability.

This trade-off can also be used to inform choices made in FDR procedures. For FDR procedures, choices that decrease the upward bias in \( \widehat{\text{FDP}} \) lead to more powerful procedures. Li and Barber (2017) show that any accumulation function bounded by \( B \) leads to the same FDR guarantee, but that among accumulation functions with the same upper bound, SeqStep leads to the least upwardly-biased FDP estimates (as suggested by the left panel of Figure 9) and thus the most powerful accumulation tests. However, our observation that SeqStep has a high FDP multiplier \( c(\alpha) \) suggests that this choice also leads to increased variance in \( \widehat{\text{FDP}} \). Indeed, the fact that SeqStep is the “steepest” accumulation function among those with a fixed maximum \( B \) implies also that

\[
h_{\text{SeqStep}} = \arg \max_{h : h \leq B} \text{Var}[h(U)].
\]

Therefore, the SeqStep accumulation test is the most powerful, but also the most variable, adding more nuance to Li and Barber’s conclusion. If we

---

**Figure 9.** Comparing \( \widehat{\text{FDP}} \) and \( \text{FDP} \) for three accumulation functions. In the left panel, the three paths of \( \widehat{\text{FDP}} \) are plotted, along with the mean \( \text{FDP} \). Flatter accumulation functions lead to larger \( \widehat{\text{FDP}} \) estimates. In the right panel, \( \text{FDP}(R_k) = c(\alpha) \cdot \widehat{\text{FDP}}(R_k) \) are shown for the three accumulation functions, along with the pointwise FDP quantiles. We see the nontrivial trade-off between \( c(\alpha) \) and \( \widehat{\text{FDP}} \), with HingeExp providing the best \( \text{FDP} \) curve.
switch from considering the mean of the FDP to its upper quantiles, then other accumulation functions are likely to more favorably trade off FDP with power. We leave this direction of inquiry for future work.

Finally, though we have used accumulation tests as an illustrations of the trade-offs between \( c(\alpha) \) and FDP, similar phenomena arise in the context of other “tuning” parameters as well.

**APPENDIX D: EXAMINING THE EFFECT OF CORRELATION**

Figure 10 shows the result of numerical simulations under AR(1) dependence for the six procedures considered before, all with \( a = 1 \). These curves all correspond to the global null case, which leads to the largest FDP multipliers. As we vary the correlation parameter \( \rho \) from \(-0.9\) to \(0.9\), we can see how the empirical quantiles change. We observe that higher correlations lead to larger FDP quantiles, as expected, but under moderate correlations these quantiles are still below or at least near the theoretical bounds under independence.

Figure 11 shows how the expectation bounds change with \( \rho \). Interestingly,
the FDR multipliers are U-shaped in $\rho$ in some settings and monotonically increasing in other settings. The bounds for $\pi_{\text{sort}}$ and $\pi_{\text{online-simple}}$ are remarkably robust to local correlation, whereas the other bounds grow somewhat more rapidly for large $\rho$. Investigating theoretically how our bounds change under correlation (and how to precisely quantify correlation) is left for future work.

![FDR Multipliers Under Correlation](image)

**Fig 11.** FDR bounds under local correlation. Most procedures seem less affected by negative correlation than by strong positive correlations. Crosses indicate multipliers for $\rho = 0$, the case with independent $p$-values as considered in the theorems of this paper.

**Eugene Katsevich**  
Department of Statistics  
Stanford University  
E-mail: ekatsevi@stanford.edu

**Aaditya Ramdas**  
Department of Statistics and Data Science  
Carnegie Mellon University  
E-mail: aramdas@cmu.edu