PROCEDURES CONTROLLING THE *k*-FDR USING BIVARIATE DISTRIBUTIONS OF THE NULL *p*-VALUES

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Abstract: Procedures controlling error rates measuring at least k false rejections, instead of at least one, are often desired while testing a large number of hypotheses. The k-FWER, probability of at least k false rejections, is such an error rate that has been introduced, and procedures controlling it have been proposed. Recently, Sarkar (2007) introduced an alternative, less conservative notion of error rate, the k-FDR, generalizing the usual notion of false discovery rate (FDR), and proposed a procedure controlling it based on the k-dimensional joint distributions of the null p-values and assuming MTP₂ (multivariate totally positive of order two) positive dependence among all the p-values. In this article, we assume a less restrictive form of positive dependence than MTP₂, and develop alternative procedures based only on the bivariate distributions of the null p-values.

Key words and phrases: Arbitrary dependence, average power, clumpy dependence, generalized FDR, multiple hypothesis testing, positive regression dependence on subset, stepwise procedure.

1. Introduction

Often in practice when a large number of null hypotheses are being simultaneously tested, one is willing to tolerate a few false rejections but wants to control the occurrence of too many of them, say k or more. The k-FWER, probability of falsely rejecting at least k null hypotheses, is an appropriate error rate in this context. A number of procedures controlling it have been proposed in the literature; see, for example, Sarkar (2008) for references. Sarkar (2007) recently proposed using the k-FDR, the expected ratio of k or more false rejections to the total number of rejections, which generalizes the false discovery rate (FDR) of Benjamini and Hochberg (1995, BH). He developed two k-FDR procedures utilizing the kth order joint null distributions of the p-values, one under independence or the MTP₂ positive dependence (Karlin and Rinott (1980)), generalizing the BH FDR procedure, and the other under any form of dependence among the p-values, generalizing the FDR procedure of Benjamini and Yekutieli (2001, BY). Sarkar and Guo (2009) also considered a mixture model involving independent p-values, and provided a simple, intuitive upper bound to the k-FDR. Based on this, they introduced conservative point estimates of the k-FDR and through them, newer stepup k-FDR procedures. The k-FDR control of these procedures was proved for independent test statistics.

Here we go back to the work of Sarkar (2007) and develop alternative k-FDR procedures relaxing both the MTP_2 condition and the use of the k-dimensional joint distributions of the null *p*-values. More specifically, we assume the positive dependence condition, a weaker version of the MTP₂, under which a stepwise procedure, stepdown or stepup, with the critical values of the BH procedure (to be simply referred to as the BH stepwise procedure) known to control the FDR (Benjamini and Yekutieli (2001) and Sarkar (2002)), and generalize this BH stepwise procedure to a k-FDR stepwise procedure based only on the bivariate distributions of the null *p*-values. The positive dependence condition assumed is slightly weaker than considered originally in the above two papers. We offer two such generalizations in the positive dependence case, one more conservative than the other but easier to implement, both reducing to the same procedure under independence. Often in practice, as in microarray analyses or fMRI studies, the *p*-values tend to be *clumpy dependent* in the sense that they are more positively dependent within small groups, strongly or weakly, but are independent between these groups. Two alternative stepwise procedures controlling the k-FDR are presented in this case.

We numerically compare each of our proposed k-FDR stepwise procedures with the corresponding BH stepwise procedure, knowing that an FDR procedure can also serve as a k-FDR procedure, albeit more conservatively, and that the minimum we expect of a k-FDR procedure is to perform better than the corresponding FDR procedure. For appropriately chosen values of k, the proposed k-FDR stepwise procedures are seen to be uniformly more powerful than the corresponding BH stepwise procedure under independence or a weak positive dependence among the p-values. With increasing positive dependence among the p-values, our k-FDR stepwise procedures unfortunately lose their edges over the corresponding FDR procedure. However, in case of clumpy dependence among the p-values, the proposed k-FDR procedures are seen to improve their performances, maintaining their power dominance over the corresponding BH stepwise procedure even under high positive dependence among the p-values.

An alternative stepdown k-FDR procedure is proposed that performs better than the stepdown part of the above stepwise procedure under independence. Finally, we develop a generalized BY procedure that uniformly outperforms the original BY procedure as a k-FDR procedure under any form of dependence.

The paper is organized as follows. With some background information and result given in Section 2, we present the developments of our k-FDR procedures under positive dependence, clumpy dependence, and independence situations in

1228

Section 3. The findings from some numerical studies on the performances of our procedures are given in Section 4. Section 5 deals with the proposed k-FDR procedure under arbitrary dependence. Most of the technical details and a graph showing the power performance of the above alternative stepdown procedure are placed as a Web Appendix in http://www.stat.sinica.edu.tw/statistica.

2. Preliminaries

Let H_1, \ldots, H_n be the null hypotheses being simultaneously tested using the corresponding *p*-values P_1, \ldots, P_n , respectively. Let $P_{(1)} \leq \cdots \leq P_{(n)}$ be the ordered *p*-values and $H_{(1)}, \ldots, H_{(n)}$ the associated null hypotheses. Then, given a non-decreasing set of critical constants $0 < \alpha_1 \leq \cdots \leq \alpha_n < 1$, a stepdown multiple testing procedure rejects the set of null hypotheses $\{H_{(i)}, i \leq i_{SD}^*\}$ and accepts the rest, where $i_{SD}^* = \max\{i : P_{(j)} \leq \alpha_j \forall j \leq i\}$ if the maximum exists, otherwise it accepts all the null hypotheses. A stepup procedure, on the other hand, rejects the set $\{H_{(i)}, i \leq i_{SU}^*\}$ and accepts the rest, where $i_{SU}^* = \max\{i : P_{(i)} \leq \alpha_i\}$ if the maximum exists, otherwise it accepts all the null hypotheses. A stepup procedure, and the null hypotheses. A stepup is constant is referred to as a single-step procedure.

The constants in a stepwise procedure are determined subject to the control at a pre-specified level α of a suitable error rate. With R and V denoting, respectively, the total numbers of rejected and falsely rejected null hypotheses, the k-FDR is defined as k-FDR = E(k-FDP), where k-FDP = V/R if $V \ge k$, and = 0 otherwise (Sarkar (2007)). The k-FDR is the expected ratio of k or more false rejections to the total number of rejections, reducing to the original FDR when k = 1. It is a less conservative notion of error rate than the FDR, as k-FDR \le FDR. Using it when one is willing to control at least k false rejections, rather than at least one, is a natural generalization of the idea of using the k-FWER $= P\{V \ge k\}$ instead of the FWER $= P\{V \ge 1\}$.

The following lemma, with proof given in the Web Appendix, is key to developing the k-FDR procedures. We assume that n_0 is the number of true null hypotheses and $\hat{P}_1, \ldots, \hat{P}_{n_0}$ are the corresponding *p*-values.

Lemma 2.1. Given a stepwise procedure involving P_1, \ldots, P_n and the critical values $0 < \alpha_1 \le \cdots \le \alpha_n < 1$, consider the corresponding stepwise procedure in terms of the null p-values $\hat{P}_1, \ldots, \hat{P}_{n_0}$ and the critical values $\alpha_{n-n_0+1} \le \cdots \le \alpha_n$. Let V_n be the number of false rejections in the stepwise procedure and \hat{R}_{n_0} be the number of rejections in the stepwise procedure involving the null p-values. Then, $\{V_n \ge k\} \subseteq \{\hat{R}_{n_0} \ge k\}$ for any fixed $k \le n_0 \le n$.

Remark 2.1. With Lemma 2.1, construction of a stepwise procedure providing a control of the k-FWER at α basically reduces to that of finding the constants in that procedure guaranteeing the inequality $P\{\hat{R}_{n_0} \geq k\} \leq \alpha$ for all $k \leq n_0 \leq n$. It unifies the arguments used separately towards constructing stepdown k-FWER and stepup k-FWER procedures in Lehmann and Romano (2005) and Romano and Shaikh (2006).

We assume that each $P_i \sim U(0, 1)$ when the corresponding H_i is true and, jointly, the *p*-values are positively dependent in the sense that

$$E\left\{\phi(P_1,\ldots,P_n) \mid \hat{P}_i \le u\right\} \uparrow u \in (0,1),$$

$$(2.1)$$

for each \hat{P}_i and any increasing (coordinatewise) function ϕ . This is slightly weaker than $E\left\{\phi(P_1,\ldots,P_n) \mid \hat{P}_i = u\right\} \uparrow u \in (0,1)$, the positive regression dependence on subset (PRDS) condition considered in Benjamini and Yekutieli (2001) and Sarkar (2002). A proof of the k-FDR control of our proposed procedure becomes easier when the present form of positive dependence is applied directly, even though relaxing the PRDS condition to the present form may not be of much importance from a practical standpoint. This condition is satisfied by the p-values arising in a number of multiple testing situations. In particular, it is satisfied by the p-values corresponding to multivariate normal test statistics with a common non-negative correlation as is considered in our numerical calculations.

We assume that k is pre-fixed, though it is important to note that a determination of it statistically when it is not given is an important issue; see Sarkar and Guo (2009) for a discussion. Since the k-FDR is 0, and hence trivially controlled, for any procedure if $n_0 < k$, we assume throughout this paper that $k \le n_0 \le n$.

3. k-FDR Procedures under Positive Dependence or Independence

In this section, we develop stepwise procedures that control the k-FDR for $k \geq 2$ using bivariate distributions of the null p-values, assumed known. To this end, we have the following theorem whose proof is in the Web Appendix.

Theorem 3.1. Consider a stepwise procedure with the critical values given by $\alpha_i = \{i \lor k\}\alpha_k/k, i = 1, ..., n, \text{ for some fixed } 2 \le k \le n \text{ and } 0 < \alpha_k < 1.$ Then for p-values satisfying (2.1) we have

$$k - \text{FDR} \le \max_{k \le n_0 \le n} \left\{ \frac{1}{k(k-1)} \sum_{i=1}^{n_0} \sum_{j(\ne i)=1}^{n_0} H_{ij}\left(\alpha_k, \frac{(n-n_0+k)\alpha_k}{k}\right) \right\} , (3.1)$$

where $H_{ij}(u,v) = P\{\hat{P}_i \leq u, \hat{P}_j \leq v\}, i \neq j$, are the bivariate cdf's of the null *p*-values.

We can apply the inequality $P\{\hat{P}_i \leq u \mid \hat{P}_j \leq v'\} \leq \{\hat{P}_i \leq u \mid \hat{P}_j \leq v\}$, for any $v \leq v'$, that characterizes the positive dependence property shared by every pair (\hat{P}_i, \hat{P}_j) , to the right-hand side in (3.1) to obtain a more relaxed, but easier to utilize, upper bound to the k-FDR than the one in Theorem 3.1.

Corollary 3.1. For the stepwise procedure in Theorem 3.1, and under the same conditions, for $k \ge 2$,

$$k \text{-FDR} \le \max_{k \le n_0 \le n} \left\{ \frac{n - n_0 + k}{k^2 (k - 1)} \sum_{i=1}^{n_0} \sum_{j(\ne i)=1}^{n_0} H_{ij}(\alpha_k, \alpha_k) \right\} .$$
(3.2)

The k-FDR of the stepwise procedure in Theorem 3.1 can be controlled at α by equating the upper bound in (3.1) or (3.2) to α and solving the resulting equation for α_k . Of course one needs to know the bivariate distributions of all pairs of null *p*-values. For instance, when the null *p*-values are exchangeable with H as the common and known bivariate cdf, the α_k can be obtained from

$$\max_{k \le n_0 \le n} \left\{ \frac{n_0(n_0 - 1)}{k(k - 1)} H\left(\alpha_k, \frac{(n - n_0 + k)\alpha_k}{k}\right) \right\} = \alpha \tag{3.3}$$

or, can be obtained more conservatively by solving

$$\frac{D(k,n)H(\alpha_k,\alpha_k)}{k^2(k-1)} = \alpha, \text{ with } D(k,n) = \max_{k \le n_0 \le n} \left\{ n_0(n_0-1)(n-n_0+k) \right\}.$$
(3.4)

Often in practice, as in microarray analysis and fMRI studies, the *p*-values tend to be *clumpy dependent* in the sense that they are more (positively) dependent within groups than between groups. Suppose that there are *g* independent groups and, for each $i = 1, \dots, n_0, J_i$ is the set of indices of null hypotheses in the group containing the \hat{P}_i . Clearly, $J_i \equiv J_j$ if *i* and *j* belong to the same group. The upper bounds in Theorem 3.1 and Corollary 3.1 can be expressed, respectively, in this case as

$$k\text{-FDR} \le \max_{k \le n_0 \le n} \left\{ \frac{n - n_0 + k}{k^2 (k - 1)} \sum_{i=1}^{n_0} \sum_{j(\ne i) \in J_i} \left[\frac{k}{n - n_0 + k} H_{ij} \left(\alpha_k, \frac{(n - n_0 + k)\alpha_k}{k} \right) + (n_0 - |J_i|) \alpha_k^2 \right] \right\},$$
(3.5)

$$k\text{-FDR} \le \max_{k \le n_0 \le n} \left\{ \frac{n - n_0 + k}{k^2 (k - 1)} \sum_{i=1}^{n_0} \sum_{j(\ne i) \in J_i} \left[H_{ij} \left(\alpha_k, \alpha_k \right) + (n_0 - |J_i|) \alpha_k^2 \right] \right\}, (3.6)$$

where $|J_i|$ is the cardinality of J_i . Stepwise procedures controlling the k-FDR in case of clumpy dependence can then be constructed by equating the upper bound in (3.5) or (3.6) to α and solving for α_k .

When the p-values are independent, we have the following.

Proposition 3.1. A stepwise procedure with the critical values $\alpha_i = (i \vee k)\beta/n$, i = 1, ..., n, with $\beta = n\sqrt{(k-1)\alpha/D(k,n)}$, controls the k-FDR at α when the *p*-values are independent.

In fact, an alternative to the stepdown part of the procedure in Proposition 3.1 can be obtained under independence. Consider a stepdown procedure with critical values $\alpha_i = \{i \lor k\}\beta/n, i = 1, ..., n$, for a fixed $0 < \beta < 1$. For this procedure, we have

$$k$$
-FDR $\leq \frac{n_0 \beta}{n} P \{ R_{n_0 - 1} \geq k - 1 \},$ (3.7)

as shown in the Web Appendix, where R_{n_0-1} is the number of rejections in the stepdown procedure based on $\hat{P}_{(1):n_0-1} \leq \cdots \leq \hat{P}_{(n_0-1):n_0-1}$, the ordered versions of any $n_0 - 1$ of the n_0 null *p*-values, and the corresponding critical values $\alpha_{n-n_0+2} \leq \cdots \leq \alpha_n$. Let

$$G_{k,n}(u) = P\left\{U_{(k)} \le u\right\} = \sum_{j=k}^{n} \binom{n}{j} u^{j} (1-u)^{n-j}$$

the cdf of the kth order statistic based on n iid U(0, 1). Then, since

$$P\{R_{n_0-1} \ge k-1\} = P\left\{\hat{P}_{1:n_0-1} \le \alpha_{n-n_0+2}, \dots, \hat{P}_{(k-1):n_0-1} \le \alpha_{n-n_0+k}\right\}$$
$$\le G_{k-1,n_0-1}(\alpha_{n-n_0+k}) ,$$

we have the following.

Proposition 3.2. Consider a stepdown procedure with the critical values $\alpha_i = (i \lor k)\beta/n$, i = 1, ..., n, where

$$\frac{\beta}{n} \max_{k \le n_0 \le n} \left\{ n_0 G_{k-1,n_0-1} \left(\frac{(n-n_0+k)\beta}{n} \right) \right\} = \alpha .$$

$$(3.8)$$

The k-FDR is controlled at α when the p-values are independent.

We show numerically in the next section that the stepdown procedure in Proposition 3.2 indeed performs better than the stepdown procedure in Proposition 3.1 under independence.

1232

Remark 3.1. In a stepwise procedure providing a control of the k-FDR, the first k - 1 critical values can be chosen arbitrarily without affecting the k-FDR, as in the case of a k-FWER stepwise procedure (Lehmann and Romano (2005) and Sarkar (2007, 2008)). Nevertheless, as argued in those papers, keeping these critical values constant at the kth critical value would be the best option. This is what we do in this paper. Thus, even though one can use the stepwise BH procedure with the critical values $\alpha_i = i\alpha/n, i = 1, \ldots, n$, as a k-FDR procedure, one may consider improving it by modifying its critical values to $\alpha_i = (i \vee k)\alpha/n$, $i = 1, \ldots, n$; we call this the k-FDR version of the stepwise BH procedure. Of course, this k-FDR BH procedure does not take full advantage of the notion of k-FDR in that its critical values are determined directly using a formula for the the FDR, not the k-FDR, and hence can potentially be improved. It is this k-FDR version of stepwise BH procedure against which we numerically investigate the performances of our proposed k-FDR procedures in the next section.

4. Simulations

We present in this section the results of simulation studies we conducted to investigate the performances of our k-FDR procedures developed under different types of dependence among the p-values – positive dependence, clumpy dependence, and independence. These studies were geared toward comparing our procedures with the k-FDR version of the BH stepwise procedure in terms of the average power, the expected proportion of false null hypotheses that are rejected. For the positive dependence case, our procedures are the ones that are based on α_k determined from the upper bound in Theorem 3.1, or its corollary. For the clumpy dependence case, these are based on the α_k in (3.5) or (3.6). In the independence case, we focused on the stepdown procedure in Proposition 3.2 to see how it actually performs in such a case as an alternative to the one in Proposition 3.1.

In all these studies, we chose n = 200 and k = 8, and generated the *p*-values from multivariate normal test statistics. These statistics have a common non-negative correlation ρ in the case of positive dependence, and are broken up into *g* independent groups with a common non-negative correlation ρ within each group in the case of clumpy dependence. For the positive and clumpy dependence cases, we decided to present the power comparisons for different degrees of dependence. However, since we had to numerically compute the critical values of our procedures for this (n, k) before proceeding to simulate their average powers, we also decided to present these critical values along with those for a variety of other choices of both n and k. This provides us a more direct comparisons between our procedures and the *k*-FDR version of the BH stepwise

Table 1. Values of β_1 and β_2 for different (n, k) and non-negative ρ with $\alpha = 0.05$.

		$\rho = 0.0$		$\rho = 0.05$		$\rho = 0.10$		$\rho = 0.15$		$\rho = 0.20$	
n	k	β_1	β_2	β_1	β_2	β_1	β_2	β_1	β_2	β_1	β_2
5	0 2	0.079	0.079	0.066	0.062	0.055	0.050	0.046	0.039	0.038	0.031
20	0 8	0.103	0.103	0.087	0.083	0.074	0.066	0.063	0.053	0.053	0.043
100	0 40	0.108	0.0108	0.092	0.087	0.078	0.070	0.066	0.056	0.056	0.045
500	0 200	0.109	0.109	0.093	0.088	0.079	0.071	0.067	0.057	0.057	0.046
1000	0 400	0.109	0.109	0.093	0.088	0.079	0.071	0.067	0.057	0.057	0.046

procedure. In the independence case, however, we consider only the average power for comparison.

We computed β , where $\alpha_k = k\beta/n$, from the upper bounds in Theorem 3.1 and its corollary, with the *p*-values assumed to be generated from multivariate normal test statistics with a common non-negative correlation ρ . Values of β for some (n, k, ρ) and $\alpha = 0.05$ are presented in Table 1, where $\beta \equiv \beta_1 =$ $n\alpha_k/k$ with α_k in (3.1), and $\beta \equiv \beta_2 = n\alpha_k/k$ with α_k in (3.2). Comparing the values of both β_1 and β_2 directly with $\alpha = 0.05$, we notice that when the *p*-values are independent or weakly but positively dependent our proposed *k*-FDR stepwise procedures are based on quite large critical values, and hence quite powerful relative to the *k*-FDR version of the corresponding stepwise BH procedure. However, as the *p*-values become more and more positively dependent, our procedures lose their edge over this *k*-FDR version of stepwise BH procedure. To see the extent of power improvement our *k*-FDR procedures offer over the *k*-FDR version of the BH procedure in case of weakly but positively dependent *p*-values, we carried out further numerical investigations in terms of the average power, but this time considering only stepup procedures.

Figure 1 presents a comparison of the simulated average powers of the stepup procedures corresponding to β_1 and β_2 , labelled k-FDR SU 1 and k-FDR SU 2, respectively, and the k-FDR version of the BH procedure, labelled k-FDR BH. The simulated average power for each procedure was obtained by (i) generating n = 200 dependent normal random variables $N(\mu_i, 1)$, $i = 1, \dots, n$, with a common correlation $\rho = 0.05, 0.1, 0.15$ or 0.2, and with n_1 of the 200 μ_i 's being equal to d = 2 and the rest 0, (ii) applying the corresponding stepup procedure with k = 8 to the generated data to test $H_i : \mu_i = 0$ against $K_i : \mu_i \neq 0$ simultaneously for $i = 1, \dots, 200$ at $\alpha = 0.05$, and (iii) repeating steps (i) and (ii) 1,000 times before observing the proportion of the n_1 false H_i 's that were correctly declared significant. The values of β_1 and β_2 for (n, k) = (200, 8) and $\rho = 0.05, 0.1, 0.15$ and 0.2 were taken from Table 1. As seen from this figure, our proposed k-FDR stepup procedures are uniformly more powerful than the

PROCEDURES CONTROLLING THE k-FDR



Figure 1. Power of two k-FDR stepup procedures in the case of positive dependence with parameters n = 200, k = 8, d = 2 and $\alpha = 0.05$.

BH stepup procedure under weak dependence, with the power difference getting significantly higher with increasing numbers of false null hypotheses.

We did similar kind of calculations for the clumpy dependence case. Table 2 presents the values of $\beta_1 = n\alpha_k/k$ with α_k in (3.5) and $\beta_2 = n\alpha_k/k$ with α_k in (3.6) for some values of (n, k, g, ρ) and $\alpha = 0.05$. This time, our stepwise procedures are seen to uniformly dominate the corresponding stepwise BH procedure even for positive correlations as large as 0.5. For correlation larger than 0.5, while the procedure corresponding to β_1 continues to uniformly dominate the corresponding to β_2 works well only when the number of null hypotheses is large. A further comparison in terms of the average power is presented in Figure 2, having simulated these powers for (n, k, g) = (200, 8, 20), $\rho = 0, 0.2, 0.5$ and 0.8, and $\alpha = 0.05$. In this graph, the stepup procedures corresponding to β_1 and β_2 and the k-FDR version of the BH procedure are labelled k-FDR SU 1, k-FDR SU 2, and k-FDR BH,



Figure 2. Power of two k-FDR stepup procedures in the case of clumpy dependence with parameters n = 200, g = 20, k = 8, d = 2 and $\alpha = 0.05$.

Table 2. Values of β_1 and β_2 for different (n, k, g) and non-negative ρ under clumpy dependence with $\alpha = 0.05$.

			$\rho = 0.0$		$\rho = 0.2$		$\rho = 0.5$		$\rho = 0.8$	
n	k	g	β_1	β_2	β_1	β_2	β_1	β_2	β_1	β_2
200	8	20	0.103	0.103	0.096	0.092	0.079	0.058	0.054	0.022
500	20	25	0.107	0.107	0.101	0.098	0.086	0.065	0.063	0.026
1000	40	40	0.108	0.108	0.105	0.102	0.094	0.078	0.076	0.038
5000	200	100	0.109	0.109	0.108	0.107	0.103	0.095	0.095	0.066
10000	400	100	0.109	0.109	0.108	0.107	0.103	0.095	0.095	0.066

respectively. Figure 2 reinforces our previous observations regarding the relative performances of these procedures made from Table 2.

Lastly, we repeated our simulation for the independence case. The average powers were simulated for the procedures in Propositions 3.2 and 3.1, and the *k*-FDR version of the stepdown BH procedure, with $(n, k, \rho) = (200, 5, 0)$ and $\alpha = 0.05$. These are presented in Web Figure 1, having labelled these procedures k-FDR SD 1, k-FDR SD 2, and k-FDR BH, respectively. We notice that the stepdown procedure in Proposition 3.2 indeed performs much better than the other two stepdown procedures under independence.

5. k-FDR Procedure under Arbitrary Dependence

We now consider developing a stepup procedure, with a control of the k-FDR under any form of dependence of the *p*-values, that will uniformly dominate the BY procedure with the critical values $\alpha_i = i\alpha/n\sum_{j=1}^n \frac{1}{j}$, $i = 1, \ldots, n$, or its modification obtained by keeping the first k-1 critical values the same as the kth one. To that end, we have the following theorem, proved in the Web Appendix.

Theorem 5.2. A stepup procedure with the critical values

$$\alpha_{i} = \frac{(i \lor k)\alpha}{n\left\{1 + \sum_{j=k+1}^{n} \frac{1}{j}\right\}}, \ i = 1, \dots, n,$$

controls the k-FDR at α .

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1238