

# A fast algorithm to compute a curve of confidence upper bounds for the False Discovery Proportion using a reference family with a forest structure

Guillermo Durand <sup>1</sup> Laboratoire de Mathématiques d'Orsay, Université Paris-Saclay

Date published: 2024-12-04 Last modified: 2024-12-04

#### **Abstract**

This paper presents a new algorithm (and an additional trick) that allows to compute fastly an entire curve of post hoc bounds for the False Discovery Proportion when the underlying bound  $V_{\Re}^*$  construction is based on a reference family  $\Re$  with a forest structure à la Durand et al. (2020). By an entire curve, we mean the values  $V_{\Re}^*(S_1), \dots, V_{\Re}^*(S_m)$  computed on a path of increasing selection sets  $S_1 \subseteq \dots \subseteq S_m$ ,  $|S_t| = t$ . The new algorithm leverages the fact that going from  $S_t$  to  $S_{t+1}$  is done by adding only one hypothesis.

*Keywords*: multiple testing, algorithmic, post hoc inference, false discovery proportion, confidence bound

#### Contents

2	1	Introduction	2
3	2	Notation and reference family methodology	3
4		2.1 Multiple testing notation	3
5		2.2 Post hoc bounds with reference families	3
6		2.3 Regions with a forest structure	4
7	3	New algorithms	8
8	9	3.1 Pruning the forest	8
9		3.2 Fast algorithm to compute a curve of confidence bounds on a path of selection sets	10
10	4	Implementation	18
11	5	Numerical experiments	19
12	6	Conclusion	19
13	7	Acknowledments	19
14	Re	eferences	19
15	Se	ession information	20

 $<sup>^{1}</sup> Corresponding\ author:\ guillermo.durand@universite-paris-saclay.fr$ 

# 1 Introduction

Multiple testing theory is often used for exploratory analysis, like Genome-Wide Association Studies,
where multiple features are tested to find promising ones. Classical multiple testing theory like
Family-Wise Error Rate (FWER) control or False Discovery Rate (FDR) control (Benjamini and
Hochberg, 1995) can be used, but a more recent trend consists in the computation of post hoc bounds,
also named post selection bounds or confidence envelopes, for the number of false positives, or,
equivalently, for the False Discovery Proportion (FDP). This approach is notably advocated for in the
context of exploratory research by (Goeman and Solari, 2011, Section 1).

Mathematically speaking, a confidence upper bound (we prefer to say upper bound instead of envelope for obvious reasons) is a function  $\hat{V}: \mathcal{P}(\mathbb{N}_m^*) \to \mathbb{N}_m$ , where  $\mathbb{N}_m = \{0, ..., m\}$ ,  $\mathbb{N}_m^* = \{1, ..., m\}$  and m is the number of hypotheses, such that

$$\forall \alpha \in ]0, 1[, \mathbb{P}\left(\forall S \subseteq \mathbb{N}_m^*, |S \cap \mathcal{H}_0| \le \hat{V}(S)\right) \ge 1 - \alpha. \tag{1}$$

Here,  $\alpha$  is a target error rate and  $\mathcal{H}_0$  is the set of hypotheses indices that are true null hypotheses. Note that the construction of  $\hat{V}$  depends on  $\alpha$  and on the random data X and the dependence is omitted to lighten notation and because there is no ambiguity. The meaning of Equation (1) is that  $\hat{V}$  provides an upper bound of the number of null hypotheses in S for any selection set  $S \subseteq \mathbb{N}_m^*$ , which allows the user to perform post hoc selection on their data without breaching the statistical guarantee. Also note that by dividing by  $|S| \vee 1$  in Equation (1) we also get a confidence bound for the FDP:

$$\forall \alpha \in ]0, 1[, \mathbb{P}\left(\forall S \subseteq \mathbb{N}_m^*, \text{FDP}(S) \le \frac{\hat{V}(S)}{|S| \vee 1}\right) \ge 1 - \alpha.$$
 (2)

So post hoc bounds provide ways to construct FDP-controlling sets instead of FDR-controlling sets, which is much more desirable given the nature of the FDR as an expected value. See for example (Bogdan et al., 2015, Figure 4) for a credible example where the FDR is controlled but the FDP has a highly undesirable behavior (either 0 because no discoveries at all are made, either higher than the target level).

The first confidence bounds are found in Genovese and Wasserman (2006) and Meinshausen (2006), although, in the latter, only for selection sets of the form  $\{i \in \mathbb{N}_m : P_i \le t\}$  where  $P_i$  is the p-value associated to the null hypothesis  $H_{0,i}$ . In Goeman and Solari (2011) the authors re-wrote the generic construction of Genovese and Wasserman (2006) in terms of closed testing Marcus et al. (1976), proposed several practical constructions and sparked a new interest in multiple testing procedures based on confidence envelopes. This work was followed by a prolific series of works like Meijer et al. (2015) or Vesely et al. (2023). In Blanchard et al. (2020), the authors introduce the new point of view of references families (see Section 2.2) to construct post hoc bounds, and show the links between this meta-technique and the closed testing one, along with new bounds.

Following the reference family trail, in Durand et al. (2020) the authors introduce new reference families with a special set-theoretic constraint that allows an efficient computation of the bound denoted by  $V_{\mathfrak{R}}^*$  on a single selection set S. The problem is that one often wants to compute  $V_{\mathfrak{R}}^*$  on a whole path of selection sets  $(S_t)_{t\in\mathbb{N}_m^*}$ , for example the hypotheses attached to the t smallest p-values. Whereas the algorithm provided in the aforementioned work (Durand et al., 2020, Algorithm 1), which is reproduced here, see Algorithm 1, is fast for a single evaluation, it is slow and inefficient to repeatedly call it to compute each  $V_{\mathfrak{R}}^*(S_t)$ . If the  $S_t$ 's are nested, and growing by one, that is  $S_1 \subseteq \cdots \subseteq S_m$  and  $|S_t| = t$ , there is a way to efficiently compute  $(V_{\mathfrak{R}}^*(S_t))_{t\in\mathbb{N}_m}$  by leveraging the nested structure

This is the main contribution of the present paper: a new and fast algorithm computing the curve  $\left(V_{\mathfrak{R}}^{*}(S_{t})\right)_{t\in\mathbb{N}_{m}}$  for a nested path of selection sets, that is presented in Section 3.2. An additional

algorithm that can speed up computations both for the single-evaluation algorithm and the new curve-evaluation algorithm is also presented, in Section 3.1. In Section 2.1, all necessary notation and vocabulary is re-introduced, most of it being the same as in Durand et al. (2020). In Section 4 we discuss the current implementations of all the presented algorithms in the R (R Core Team, 2020) package sanssouci (Neuvial et al., 2024). Finally, a few numerical experiments are presented in Section Section 5 to demonstrate the computation time gain.

# 4 2 Notation and reference family methodology

#### 5 2.1 Multiple testing notation

As is usual in multiple testing theory, we consider a probability space  $(\Omega, \mathcal{A}, \mathbb{P})$ , a model  $\mathscr{P}$  on a measurable space  $(\mathcal{X}, \mathfrak{X})$ , and data that is represented by a random variable  $X : (\Omega, \mathcal{A}) \to (\mathcal{X}, \mathfrak{X})$  with  $X \sim P \in \mathscr{P}$ , that is, the law of X is comprised in the model  $\mathscr{P}$ .

Then we consider  $m \geq 1$  null hypotheses  $H_{0,1}, \ldots, H_{0,m}$  which formally are submodels, that is subsets of  $\mathscr{P}$ . The associated alternative hypotheses  $H_{1,1}, \ldots, H_{1,m}$  are submodels such that  $H_{0,i} \cap H_{1,i} = \emptyset$  for all  $i \in \mathbb{N}_m^*$ . We denote by  $\mathscr{H}_0 = \mathscr{H}_0(P)$  (the dependence in P will be dropped when there is no ambiguity) the set of all null hypotheses that are true, that is  $\mathscr{H}_0(P) = \{i \in \mathbb{N}_m^* : P \in H_{0,i}\}$ . In other words,  $H_{0,i}$  is true if and only if  $i \in \mathscr{H}_0$ . For testing each  $H_{0,i}, i \in \mathbb{N}_m^*$ , we have at hand a p-value  $p_i = p_i(X)$  (the dependence in X will be dropped when there is no ambiguity) which is a random variable with the following property: if  $i \in \mathscr{H}_0$ , then the law of  $p_i$  is super-uniform, which is sometimes denoted  $\mathscr{L}(p_i) \succeq \mathscr{U}([0,1])$ . This means that in such case, the cumulative distribution function (cdf) of  $p_i$  is always smaller than or equal to the cdf of a random variable  $U \sim \mathscr{U}([0,1])$ :

$$\forall x \in \mathbb{R}, \mathbb{P}(p_i \le x) \le \mathbb{P}(U \le x) = 0 \lor (x \land 1). \tag{3}$$

For every subset of hypotheses  $S \subseteq \mathbb{N}_m^*$ , let  $V(S) = |S \cap \mathcal{H}_0|$ . If we think of S as a selection set of hypotheses deemed significant, V(S) is then the number of false positives (FP) in S. V(S) is our main object of interest and the quantity that we wish to over-estimate with confidence upper bounds (see Equation (1) or the more formal Equation (4) below).

Finally let us consider the following toy example, that will be re-used in the remainder of the paper.

Example 2.1 (Gaussian one-sided). In this case we assume that  $X = (X_1, ..., X_m)$  is a Gaussian vector and the null hypotheses refer to the nullity of the means in contrast to their positivity. That is, formally,  $(\mathcal{X}, \mathfrak{X}) = (\mathbb{R}^m, \mathcal{B}(\mathbb{R}^m))$ ,  $\mathscr{P} = \{\mathcal{N}(\boldsymbol{\mu}, \Sigma) : \forall j \in \mathbb{N}_m^*, \mu_j \geq 0, \Sigma \text{ positive semidefinite}\}$ , for each  $i \in \mathbb{N}_m^*$ ,  $H_{0,i} = \{\mathcal{N}(\boldsymbol{\mu}, \Sigma) \in \mathscr{P} : \mu_i = 0\}$  and  $H_{1,i} = \{\mathcal{N}(\boldsymbol{\mu}, \Sigma) \in \mathscr{P} : \mu_i > 0\}$ . Then we can construct p-values by letting  $p_i(X) = \bar{\Phi}(X_i) = 1 - \Phi(X_i)$ , where  $\Phi$  denotes the cdf of  $\mathcal{N}(0, 1)$  and  $\bar{\Phi}$  the associated survival function.

#### 2.2 Post hoc bounds with reference families

With the formalism introduced in last section, a confidence upper bound is a functional  $\hat{V}: \mathcal{X} \times ]0,1[ \to (\mathcal{P}(\mathbb{N}_m^*) \to \mathbb{N}_m)$  such that,

$$\forall P \in \mathcal{P}, \forall X \sim P, \forall \alpha \in ]0, 1[, \mathbb{P}\left(\forall S \subseteq \mathbb{N}_m^*, V(S) \le \hat{V}(X, \alpha)(S)\right) \ge 1 - \alpha. \tag{4}$$

In the remainder, the dependence in  $(X, \alpha)$  will be dropped when there is no ambiguity and  $\hat{V}(X, \alpha)$  will simply be written  $\hat{V}$ .

As said in the Introduction, many constructions, ultimately theoretically equivalent but differing by the practical steps involved, exist, and in this paper we focus on the meta-construction of Blanchard et al. (2020) based on reference families. A reference family is a family  $\Re = \Re(X,\alpha) = (R_k,\zeta_k)_{k\in\mathscr{K}}$ with  $|\mathscr{K}| \leq 2^m$ ,  $R_k \subseteq \mathbb{N}_m^*$ ,  $\zeta_k \in \{0,\dots,|R_k|\}$  where everything (that is,  $\mathscr{K}$  and all the  $R_k$  and  $\zeta_k$ ) depends on  $(X,\alpha)$  but the dependency is not explicitly written. The  $R_k$  are all distinct. We also define the following error criterion for a reference family, named Joint Error Rate (JER):

$$JER(\Re) = \mathbb{P}\left(\exists k \in \mathcal{K}, |R_k \cap \mathcal{H}_0| > \zeta_k\right) = \mathbb{P}\left(\exists k \in \mathcal{K}, V(R_k) > \zeta_k\right). \tag{5}$$

In the following, we are only interested in reference families that control the JER at level  $\alpha$ :

$$\forall P \in \mathcal{P}, \forall X \sim P, \forall \alpha \in ]0, 1[, 1 - \text{JER}(\Re(X, \alpha)) = \mathbb{P}(\forall k \in \mathcal{K}, V(R_k) \le \zeta_k) \ge 1 - \alpha. \tag{6}$$

Note that Equation (6) is really similar to Equation (4) except that the uniform guarantee, instead of being over all  $S \subseteq \mathbb{N}_m^*$ , is only over all the  $R_k \subseteq \mathbb{N}_m^*$ ,  $k \in \mathcal{K}$ , with  $\mathcal{K}$  having cardinality potentially much smaller than  $2^m$ . A global confidence bound is then derived from a JER-controlling reference family by interpolation. Let

$$\mathscr{A}(\mathfrak{R}) = \{ A \subseteq \mathbb{N}_m^* : \forall k \in \mathscr{K}, |R_k \cap A| \le \zeta_k \}. \tag{7}$$

What says the JER control is that  $\mathcal{H}_0 \in \mathcal{A}(\mathfrak{R})$ . We leverage this information with the following confidence bound construction:

$$V_{\mathfrak{R}}^{\star}(S) = \max_{A \in \mathscr{A}(\mathfrak{R})} |S \cap A| \tag{8}$$

which optimally uses the information provided by the JER control of the reference family, as proven by Proposition 2.1 of Blanchard et al. (2020). Because of the  $\max_{A \in \mathscr{A}(\Re)}$ , the computation of  $V_{\Re}^*(S)$ is generally intractable (see Proposition 2.2 of Blanchard et al. (2020)), but for specific structures of reference families, a polynomial computation can be derived. This is the topic of Durand et al. (2020) and of next section.

#### 2.3 Regions with a forest structure

112

The core concept of this section is to assume that the regions  $R_k$ 's of the reference family are what we called in Durand et al. (2020) a forest structure, that is two regions are either disjoint or nested:

$$\forall k, k' \in \mathcal{K}, R_k \cap R_{k'} \in \{R_k, R_{k'}, \emptyset\}. \tag{9}$$

Representing the  $R_k$ 's with a directed graph, where there is an oriented edge  $R_k \leftarrow R_{k'}$  if and only if  $R_k \subset R_{k'}$  and there is no  $R_{k''}$  such that  $R_k \subseteq R_{k''} \subseteq R_{k'}$  gives a forest, hence the name. See Example 2.2 and its representation in Figure 1.

We also need to introduce the notion of depth with the following function:

$$\phi : \begin{cases} \mathcal{K} \to \mathbb{N}^* \\ k \mapsto 1 + |\{k' \in \mathcal{K} : R_k \subseteq R_{k'}\}|. \end{cases}$$
 (10)

 $\{5, ..., 10\}, R_6 = \{11, ..., 16\}, R_7 = \{17, ..., 20\}, R_8 = \{21, 22\}, R_9 = \{22\}.$  This is the same example as Example 2 of Durand et al. (2020) and it is graphically depicted in Figure 1. The sets  $R_1$ ,  $R_8$  are of depth 1; the sets  $R_2$ ,  $R_3$ ,  $R_4$ ,  $R_9$  are of depth 2; the sets  $R_5$ ,  $R_6$ ,  $R_7$  are of depth 3.

Another tool of Durand et al. (2020) that will be used is its Lemma 2, that is the identification of  $\Re$  with a set  $\mathscr{C} \subset \{(i,j) \in (\mathbb{N}_N^*)^2 : i \leq j\}$  such that for  $(i,j), (i',j') \in \mathscr{C}, \{i,...,j\} \cap \{i',...,j'\} \in \{\emptyset, \{i,...,j\}, \{i',...,j'\}\}$ . With this identification, each  $R_k = R_{(i,j)}$  can be written as  $P_{i:j} = \bigcup_{i \leq n \leq j} P_n$  where  $(P_n)_{1 \leq n \leq N}$  is a partition of  $\mathbb{N}_m^*$ . The  $P_n$ 's were called atoms in Durand et al. (2020) because they have the thinnest granularity in the structure, but to continue the analogy with graphs, forests and trees, they can also be called leafs. See Example 2.3 for a concrete example.

**Example 2.2.** Let m = 25,  $R_1 = \{1, ..., 20\}$ ,  $R_2 = \{1, 2\}$ ,  $R_3 = \{3, ..., 10\}$ ,  $R_4 = \{11, ..., 20\}$ ,  $R_5 = \{1, 2\}$ 

```
%%| filename: ../figure-tikz/fig-tikz-01
\begin{tikzpicture} [scale=0.85]
 \tikzstyle{quadri}=[circle,draw,text=black, thick]
 \tikzstyle{estun}=[->,>=latex,very thick]
 \node[quadri] (R1) at (0,3) {$R_1$};
 \node[quadri] (R2) at (-2,1) {$R_2$};
 \node[quadri] (R3) at (0,1) {$R 3$};
 \node[quadri] (R4) at (2,1) {$R_4$};
 \node[quadri] (R5) at (0,-1) {$R_5$};
 \node[quadri] (R6) at (1.5,-1) {$R_6$};
 \node[quadri] (R7) at (2.5,-1) {$R 7$};
 \node[quadri] (R8) at (4,3) {$R_8$};
 \node[quadri] (R9) at (4,1) {$R_9$};
 \draw[estun] (R1)--(R2);
 \draw[estun] (R1)--(R3);
 \draw[estun] (R1)--(R4);
 \draw[estun] (R3)--(R5);
 \draw[estun] (R4)--(R6);
 \draw[estun] (R4)--(R7);
 \draw[estun] (R8)--(R9);
\end{tikzpicture}
```

Figure 1: The regions of Example 2.2.

Example 2.3 (Continuation of Example 2.2). For the reference family given in Example 2.2, a partition of atoms is given by  $P_1 = R_2$ ,  $P_2 = R_3 \setminus R_5$ ,  $P_3 = R_5$ ,  $P_4 = R_6$ ,  $P_5 = R_7$ ,  $P_6 = R_8 \setminus R_9$ ,  $P_7 = R_9$ ,  $P_8 = \mathbb{N}_m^* \setminus \{R_1 \cup R_8\}$ . Then  $R_1 = P_{1:5}$ ,  $R_3 = P_{2:3}$ ,  $R_4 = P_{4:5}$  and  $R_8 = P_{6:7}$ . Note that not all atoms are regions of the family. Those new labels are graphically depicted in Figure 2. The nodes that correspond to atoms that are not in the family are depicted with a dashed circle. This is the same example as Example 3 of Durand et al. (2020).

When all leaves are regions of the family, it is said that the family is complete. If this is not the case, the family can easily be completed by adding the missing leaves (and using their cardinality as associated  $\zeta$ ) without changing the value  $V_{\mathfrak{R}}^*$ . See Definition 2, Lemma 6 and Algorithm 2 of Durand et al. (2020) for the details.

Durand et al. (2020) also proved in their Theorem 1 that:

$$V_{\mathfrak{R}}^{\star}(S) = \min_{Q \subseteq \mathcal{X}} \left( \sum_{k' \in Q} \zeta_{k'} \wedge |S \cap R_{k'}| + \left| S \setminus \bigcup_{k' \in Q} R_{k'} \right| \right)$$
(11)

and, even better, in their Corollary 1 (iii) that:

$$V_{\mathfrak{R}}^{\star}(S) = \min_{Q \in \mathfrak{P}} \sum_{k' \in Q} \zeta_{k'} \wedge |S \cap R_{k'}|, \tag{12}$$

provided that the family is complete. Here,  $\mathfrak{P} \subseteq \mathscr{P}(\mathscr{K})$  is the set of subsets of  $\mathscr{K}$  that realize a partition, that is, the set of  $Q \subseteq \mathscr{K}$  such that the  $R_k$ ,  $k \in Q$ , form a partition of  $\mathbb{N}_m^*$ . So the minimum in Equation (12) is over way less elements than in Equation (11).

Finally, that paper provides a polynomial algorithm to  $V_{\mathfrak{R}}^*(S)$  for a single  $S \subseteq \mathbb{N}_m^*$ , which we reproduce here in Algorithm 1. The family is assumed complete, otherwise the first step would be to complete it. In the original paper,  $\mathscr{K}^h$  used to designate the elements of  $\mathscr{K}$  at depth h plus the atoms at depth

```
%%| filename: ../figure-tikz/fig-tikz-02
\begin{tikzpicture}[scale=0.85]
 \tikzstyle{quadri}=[circle,draw,text=black,thick]
 \tikzstyle{estun}=[->,>=latex,very thick]
 \node[quadri] (R1) at (0,3) {$P_{1:5}$};
 \node[quadri, fill=gray!25] (R2) at (-2,1) {$P_1$};
 \node[quadri] (R3) at (0,1) {$P_{2:3}$};
 \node[quadri] (R4) at (2,1) {$P_{4:5}$};
 \node[quadri, dashed,fill=gray!25] (P2) at (-0.5,-1) {$P_2$};
 \node[quadri,fill=gray!25] (R5) at (0.5,-1) {$P_3$};
 \node[quadri,fill=gray!25] (R6) at (1.5,-1) {$P_4$};
 \node[quadri,fill=gray!25] (R7) at (2.5,-1) {$P_5$};
 \node[quadri] (R8) at (4,3) {$P_{6:7}$};
 \node[quadri,dashed,fill=gray!25] (P6) at (3.5,1) {$P_6$};
 \node[quadri,fill=gray!25] (R9) at (4.5,1) {$P_7$};
 \node[quadri,dashed,fill=gray!25] (P8) at (6,3) {$P_8$};
 \draw[estun] (R1)--(R2);
 \draw[estun] (R1)--(R3);
 \draw[estun] (R1)--(R4);
 \draw[estun] (R3)--(R5);
 \draw[estun,dashed,thick] (R3)--(P2);
 \draw[estun] (R4) -- (R6);
 \draw[estun] (R4)--(R7);
 \draw[estun] (R8)--(R9);
 \draw[estun,dashed,thick] (R8)--(P6);
\end{tikzpicture}
```

Figure 2: The regions of Example 2.2 but with the labels of Example 2.3.

 $\leq h$ . Actually one can realize that the last assumption is not needed for this algorithm to perform exactly the same, with the added benefit of not repeating computations at the atoms that don't have the maximal depth. The only change is that sometimes  $Succ_k$  can be empty, in which case we simply let  $newVec_k = \zeta_k \wedge |S \cap R_k|$ . Thus, here in this paper, we define  $\mathcal{K}^h$  as only the elements of  $\mathcal{K}$  at depth h (the previous intricate definition may still be necessary for the proof of Theorem 1 of Durand et al. (2020)):  $\mathcal{K}^h = \{(i,j) \in \mathcal{K} : \phi(i,j) = h\}, \quad h \geq 1$ . This is the only deviation from the notation of Durand et al. (2020). Finally note that in the ongoing analogy with graph theory, the elements of  $\mathcal{K}^1$  are the roots of the different trees making up the forest.

# **Algorithm 1** Computation of a given $V_{\mathfrak{R}}^*(S)$

```
1: procedure VSTAR(S, \Re = (R_k, \zeta_k)_{k \in \mathscr{K}} with \Re complete)
 2:
            H \leftarrow \max_{k \in \mathcal{K}} \phi(k)
                                                                                                                                        ⊳ maximum depth
            for h = H - 1, ..., 1 do
 3:
                   \mathcal{K}^h \leftarrow \{k \in \mathcal{K} : \phi(k) = h\}
  4:
                   newVec \leftarrow (0)_{k \in \mathcal{K}^h}
  5:
                  for k \in \mathcal{K}^h do
  6:
                         Succ_k \leftarrow \{k' \in \mathcal{K}^{h+1} : R_{k'} \subseteq R_k\}
 7:
                         if Succ_k = \emptyset then
 8:
                               newVec_k \leftarrow \zeta_k \wedge |S \cap R_k|
 9:
10:
                               newVec_k \leftarrow \min \left( \zeta_k \wedge |S \cap R_k|, \sum_{k' \in Succ_k} Vec_{k'} \right)
11:
                         end if
12:
                   end for
13:
                   Vec \leftarrow newVec
14:
            end for
15:
            return \sum_{k \in \mathcal{K}^1} Vec_k
16:
17: end procedure
```



155

156

157

159

160

In the practical implementation of this algorithm (and of the following Algorithm 2), Vec and newVec are always of size N (the number of leaves) instead of the cardinality of  $\mathcal{K}^h$ . And the sum  $\sum_{k' \in Succ_k} Vec_{k'}$  is really easy to compute: if  $R_k = R_{(i_0,i_p-1)} = \bigcup_{j=1}^p R_{(i_{j-1},i_j-1)} = \bigcup_{i_0 \le n \le i_p-1} P_n \in \mathcal{K}^h$  for some  $p \ge 2$ , a strictly increasing sequence  $(i_0,\dots,i_p)$  and  $R_{(i_{j-1},i_{j-1})} \in \mathcal{K}^{h+1}$  for all  $1 \le j \le p$ , then we simply sum Vec over the indices from  $i_0$  to  $i_p-1$ . After that, the computed quantity is set in newVec at index  $i_0$ . So actually computing  $Succ_k$  is not needed and not done.

The computation time of the algorithm is in  $O(m|\mathcal{K}|)$ , which is fast for a single evaluation, but calling it repeatedly on a path of selection sets  $(S_t)_{t \in \mathbb{N}_m^*}$  has complexity  $O(m^2|\mathcal{K}|)$  which is not desirable and makes computations difficult in practice, hence the need for a new, faster algorithm.

Remark 2.1. The specific computation of the  $R_k$ 's and the  $\zeta_k$ 's such that Equation (6) holds is outside the scope of the present paper, but different constructions can be found in Blanchard et al. (2020), Durand et al. (2020) or Blain et al. (2022) for example.

# 3 New algorithms

#### 3.1 Pruning the forest

We remark the simple fact that if, for example,  $(1,1),(2,2),(1,2) \in \mathcal{K}$ , and  $\zeta_{(1,2)} \geq \zeta_{(1,1)} + \zeta_{(2,2)}$ , then  $R_{(1,2)}$  never contributes to the computation of any  $V_{\mathfrak{R}}^*(S)$  and it could just be removed from  $\mathfrak{R}$ . We now formalize and prove this pruning scheme.

Definition 3.1 (Pruning). We define by  $\mathcal{K}^{\mathfrak{pr}}$  ( $\mathcal{K}$  pruned) the set of elements of  $\mathcal{K}$  such that we removed all (i,i') such that there exists  $p \geq 2$  and integers  $i_1,\ldots,i_{p-1}$  such that, when setting  $i_0=i$  and  $i_p=i'+1$ , the sequence  $(i_0,\ldots,i_p)$  is strictly increasing,  $(i_{j-1},i_j-1)\in\mathcal{K}$  for all  $1\leq j\leq p$  and finally  $\zeta_{(i,i')}=\zeta_{(i_0,i_p-1)}\geq \sum_{j=1}^p\zeta_{(i_{j-1},i_j-1)}$ .

An important note is that for a removed  $(i,i') \in \mathcal{K} \setminus \mathcal{K}^{\mathfrak{pr}}$ , we can always choose the indices  $i_1, \dots, i_{p-1}$  such that actually  $(i_j, i_{j+1} - 1) \in \mathcal{K}^{\mathfrak{pr}}$  and not only  $\mathcal{K}$ , because if  $(i_j, i_{j+1} - 1) \in \mathcal{K} \setminus \mathcal{K}^{\mathfrak{pr}}$  it can itself be fragmented, and this decreasing recursion eventually ends (the later possible being at the atoms of the forest structure). Also note that removing elements from  $\mathcal{K}$  does not alter the fact that we have at hand a forest structure, that is, the reference family defined by  $\mathfrak{R}^{\mathfrak{pr}} = (R_k, \zeta_k)_{k \in \mathcal{K}^{\mathfrak{pr}}}$  has a forest structure. Because pruning a forest structure does not touch the atoms, note finally that if  $\mathcal{K}$  is complete then so is  $\mathcal{K}^{\mathfrak{pr}}$ .

178 The following proposition states that pruning the forest does not alter the bound.

Proposition 3.1. For any  $S \subseteq \mathbb{N}_m^*$ ,  $V_{\mathfrak{R}}^*(S) = V_{\mathfrak{R}^{\operatorname{pr}}}^*(S)$ .

Proof. Recall Equation (11) and, because  $\Re^{\mathfrak{pr}}$  also has a forest structure,

$$V_{\mathfrak{R}^{\flat_{\Gamma}}}^{\star}(S) = \min_{Q \subseteq \mathcal{K}^{\flat_{\Gamma}}} \left( \sum_{k' \in Q} \zeta_{k'} \wedge |S \cap R_{k'}| + \left| S \setminus \bigcup_{k' \in Q} R_{k'} \right| \right), \tag{13}$$

so we immediately get that  $V_{\mathfrak{R}}^*(S) \leq V_{\mathfrak{R}^{\mathfrak{pr}}}^*(S)$ .

Let any  $Q \subseteq \mathcal{H}$ . We split Q in A elements of  $\mathcal{H} \setminus \mathcal{H}^{\mathfrak{pr}}$ , denoted  $(i_{0,a},i_{p_a,a}-1), 1 \leq a \leq A$  for some  $p_a \geq 2$ , and B elements of  $\mathcal{H}^{\mathfrak{pr}}$ , simply denoted  $k_b$ ,  $1 \leq b \leq B$ . By the definition of  $\mathcal{H}^{\mathfrak{pr}}$  and the previous remarks, for any  $1 \leq a \leq A$ , there exist integers  $i_{1,a},\ldots,i_{p_a-1,a}$  such that  $i_{0,a} < i_{1,a} < \cdots < i_{p_a-1,a} < i_{p_a,a}$ ,  $(i_{j-1,a},i_{j,a}-1) \in \mathcal{H}^{\mathfrak{pr}}$  for all  $1 \leq j \leq p_a$ , and  $\zeta_{(i_{0,a},i_{p_a,a}-1)} \geq \sum_{j=1}^{p_a} \zeta_{(i_{j-1,a},i_{j,a}-1)}$ . Now let

$$Q^{\mathfrak{pr}} = \{k_b : 1 \le b \le B\} \cup \{(i_{j-1,a}, i_{j,a} - 1) : 1 \le a \le A, 1 \le j \le p_a\}. \tag{14}$$

We have that  $Q^{\mathfrak{pr}} \subseteq \mathscr{K}^{\mathfrak{pr}}$  and  $\bigcup_{k \in Q} R_k = \bigcup_{k \in Q^{\mathfrak{pr}}} R_k$ . Then,

$$\begin{split} \sum_{k \in Q} \zeta_k \wedge |S \cap R_k| + \left| S \setminus \bigcup_{k \in Q} R_k \right| &= \sum_{b=1}^B \zeta_{k_b} \wedge |S \cap R_{k_b}| \\ &+ \sum_{a=1}^A \zeta_{(i_{0,a}, i_{p_a,a}-1)} \wedge |S \cap R_{(i_{0,a}, i_{p_a,a}-1)}| \\ &+ \left| S \setminus \bigcup_{k \in Q} R_k \right|, \end{split}$$

but for all  $1 \le a \le A$ ,

$$\zeta_{(i_{0,a},i_{p_a,a}-1)} \ge \sum_{j=1}^{p_a} \zeta_{(i_{j-1,a},i_{j,a}-1)} 
\ge \sum_{j=1}^{p_a} \zeta_{(i_{j-1,a},i_{j,a}-1)} \wedge |S \cap R_{(i_{j-1,a},i_{j,a}-1)}|,$$

so the term  $\sum_{a=1}^{A} \zeta_{(i_{0,a},i_{p_a,a}-1)} \wedge |S \cap R_{(i_{0,a},i_{p_a,a}-1)}|$  is greater than or equal to

$$\sum_{a=1}^{A} \left( \sum_{j=1}^{p_a} \zeta_{(i_{j-1,a},i_{j,a}-1)} \wedge |S \cap R_{(i_{j-1,a},i_{j,a}-1)}| \right) \wedge |S \cap R_{(i_{0,a},i_{p_a,a}-1)}|,$$

which is simply equal to

$$\sum_{a=1}^{A} \sum_{j=1}^{p_a} \zeta_{(i_{j-1,a},i_{j,a}-1)} \wedge |S \cap R_{(i_{j-1,a},i_{j,a}-1)}|.$$

Furthermore  $\left|S \setminus \bigcup_{k \in Q} R_k \right| = \left|S \setminus \bigcup_{k \in Q^{\mathfrak{pr}}} R_k \right|$  so finally:

$$\sum_{k \in Q} \zeta_k \wedge |S \cap R_k| + \left| S \setminus \bigcup_{k \in Q} R_k \right| \ge \sum_{k \in Q^{\mathfrak{pr}}} \zeta_k \wedge |S \cap R_k| + \left| S \setminus \bigcup_{k \in Q^{\mathfrak{pr}}} R_k \right|$$

$$\ge V_{\mathfrak{M}^{\mathfrak{pr}}}^*(S).$$
(15)

Note that Equation (15) is true even if there are some  $b \in \{1, ..., B\}, a \in \{1, ..., A\}, j \in \{1, ..., p_a\}$  such that  $k_b = (i_{j-1,a}, i_{j,a} - 1)$ . We minimize over all Q to get that  $V_{\Re}^*(S) \ge V_{\Re \operatorname{pr}}^*(S)$ .  $\square$ 

This gives a practical way to speed up computations by first pruning the family before computing any  $V_{\Re}^*(S)$ , because  $\mathscr{K}^{\mathfrak{pr}}$  is smaller than  $\mathscr{K}$ , and by the above Proposition there is no theoretical loss in doing so.

Furthermore, pruning can be done really simply by following Algorithm 1 for  $S = \mathbb{N}_m^*$ , and pruning when appropriate. This gives the following Algorithm 2, assuming, for simplicity, that the family is complete. The computation time of the algorithm is the same as Algorithm 1, that is  $O(m|\mathcal{K}|)$ . Note that the only differences between Algorithm 2 and Algorithm 1 are the pruning step and  $\zeta_k$  replacing  $\zeta_k \wedge |S \cap R_k|$ , because  $\zeta_k \leq |R_k|$  and here  $S = \mathbb{N}_m^*$ , so  $\zeta_k \wedge |\mathbb{N}_m^* \cap R_k| = \zeta_k$ . Also note that the algorithm returns  $V_{\Re}^*(\mathbb{N}_m^*)$  as a by-product. The following proposition states that Algorithm 2 indeed produces the pruned region as in Definition 3.1.

**Proposition 3.2.** The final  $\mathscr{L}$  returned by Algorithm 2 is equal to  $\mathscr{K}^{\mathfrak{pr}}$ :  $\mathscr{L} = \mathscr{K}^{\mathfrak{pr}}$ .

Proof. First,  $\mathscr{K} \setminus \mathscr{L} \subseteq \mathscr{K} \setminus \mathscr{K}^{\mathfrak{pr}}$  is trivial: a k such that  $\zeta_k \geq \sum_{k' \in Succ_k} Vec_{k'}$  obviously satisfies the condition of Definition 3.1 to be pruned.

Now let  $(i,i') \in \mathcal{K} \setminus \mathcal{K}^{\mathfrak{pr}}$  an element that is pruned by Definition 3.1, so there exists  $p \geq 2$  and integers  $i_1, \dots, i_{p-1}$  such that, when setting  $i_0 = i$  and  $i_p = i' + 1$ , the sequence  $(i_0, \dots, i_p)$  is strictly increasing,  $(i_{j-1}, i_j - 1) \in \mathcal{K}$  for all  $1 \leq j \leq p$  and finally  $\zeta_{(i,i')} = \zeta_{(i_0,i_{p}-1)} \geq \sum_{j=1}^p \zeta_{(i_{j-1},i_{j}-1)}$ . Then by the proof of Theorem 1 of Durand et al. (2020) but applied to  $S = R_{(i,i')}$  we have that  $\sum_{j=1}^p \zeta_{(i_{j-1},i_{j}-1)} \geq \sum_{k' \in Succ_{(i,i')}} Vec_{k'} \text{ (see the unnumbered line just above Equation (A4) in that paper)}$  and so  $\zeta_{(i,i')} \geq \sum_{k' \in Succ_{(i,i')}} Vec_{k'}$  hence (i,i') is pruned by Algorithm 2 and  $\mathcal{K} \setminus \mathcal{K}^{\mathfrak{pr}} \subseteq \mathcal{K} \setminus \mathcal{L}$ .

In the end, 
$$\mathscr{K} \setminus \mathscr{K}^{\mathfrak{pr}} = \mathscr{K} \setminus \mathscr{L}$$
 so  $\mathscr{K}^{\mathfrak{pr}} = \mathscr{L}$ .  $\square$ 

#### Algorithm 2 Pruning of R

213

217

219

222

223

224

```
procedure Pruning(\Re = (R_k, \zeta_k)_{k \in \mathcal{X}} with \Re complete)
 2:
            H \leftarrow \max_{k \in \mathcal{K}} \phi(k)
                                                                                                                                           ⊳ maximum depth
 3:
             for h = H - 1, ..., 1 do
 4:
                   \mathcal{K}^h \leftarrow \{k \in \mathcal{K} : \phi(k) = h\}
  5:
                   newVec \leftarrow (0)_{k \in \mathcal{K}^h}
 6:
                   for k \in \mathcal{K}^h do
 7:
                         Succ_k \leftarrow \{k' \in \mathcal{K}^{h+1} \, : \, R_{k'} \subseteq R_k\}
 8:
                         if Succ_k = \emptyset then
 9:
                                newVec_k \leftarrow \zeta_k
10:
                         else
11:
                               if \zeta_k \geq \sum_{k' \in Succ_k} Vec_{k'} then
12:
                                      \mathscr{L} \leftarrow \mathscr{L} \setminus \{k\}
                                                                                                           \triangleright pruning of the region indexed by k
13:
14:
                               newVec_k \leftarrow \min\left(\zeta_k, \sum_{k' \in Succ_k} Vec_{k'}\right)
15:
                         end if
16:
                   end for
17:
                   Vec \leftarrow newVec
18:
             end for
19:
             return (\mathcal{L}, \sum_{k \in \mathcal{K}^1} Vec_k)
20:
21: end procedure
```

# 3.2 Fast algorithm to compute a curve of confidence bounds on a path of selection sets

Let  $(i_1, ..., i_m)$  a permutation of  $\mathbb{N}_m^*$ , eventually random, and, for all  $t \in \mathbb{N}_m^*$ , let  $S_t = \{i_1, ..., i_t\}$  and  $S_0 = \emptyset$ . For example,  $(i_1, ..., i_m)$  can be the permutation ordering the p-values in increasing order and in that case  $S_t$  becomes the set of indices of the t smallest p-values. Assume that we want to compute all  $V_{\Re}^*(S_t)$  for all  $t \in \{0, ..., m\}$ , this is what we call the curve of confidence bounds indexed by  $(i_1, ..., i_m)$ . Applying Algorithm 1 to compute  $V_{\Re}^*(S_t)$  for a given t has complexity  $O(t|\mathcal{K}|)$ , so using it to sequentially compute the full curve has complexity  $O(\sum_{t=0}^m t|\mathcal{K}|) = O(m^2|\mathcal{K}|)$ . In this section, we present a new algorithm that computes the curve with a  $O(m|\mathcal{K}|)$  complexity. The algorithm will need that  $\Re$  is complete, so if that is not the case we first need to complete  $\Re$  following the Algorithm 2 of Durand et al. (2020), which has a  $O(m|\mathcal{K}|)$  complexity. In the remainder of this section we assume that  $\Re$  is complete.

We first recall and introduce some notation. Recall that  $\phi$  is the depth function inside of  $\Re$ , that  $\mathfrak{P}\subseteq \mathscr{P}(\mathscr{K})$  is the set of subsets of  $\mathscr{K}$  that realize a partition, recall the important result stated by Equation (12), and that  $\mathscr{K}^h=\{k\in\mathscr{K}:\phi(k)=h\}$  for all  $1\leq h\leq H$  where  $H=\max_{k\in\mathscr{K}}\phi(k)$ . For any  $t\in\mathbb{N}_m^*$  and  $1\leq h\leq H$ , we denote by  $k^{(t,h)}$  the element of  $\mathscr{K}^h$  such that  $i_t\in R_{k^{(t,h)}}$  if it exists, and we denote by  $h_{\max}(t)$  the highest h such that  $k^{(t,h)}$  exists.

Example 3.1 (Continuation of Example 2.2 and Example 2.3). Assume that the reference family of Example 2.2 has been labeled as in Example 2.3 and completed. Let  $(i_1, ..., i_{25})$  such that  $i_1 = 7, i_2 = 1$  and  $i_3 = 24$ . Then for  $t = 1, k^{(t,1)} = (1,5), k^{(t,2)} = (2,3), k^{(t,3)} = (3,3)$  and  $h_{\max}(t) = H = 3$ . For t = 2,  $k^{(t,1)} = (1,5), k^{(t,2)} = (1,1), k^{(t,3)}$  does not exist and  $h_{\max}(t) = 2$ . For  $t = 3, k^{(t,1)} = (8,8), k^{(t,2)}$  does not exist and  $h_{\max}(t) = 1$ .

Now we can finally present the new algorithm and the proof that it computes the curve  $(V_{\mathfrak{R}}^*(S_t))_{t \in \mathbb{N}_m}$ . We present two versions of the algorithm (strictly equivalent): one very formal ( Algorithm 3 ), to

introduce additional notation used in the proof, and, later, one that is more akin to Algorithm 1 and Algorithm 2, that is, it reuses notation from step to step, for implementation and simplicity purposes (Algorithm 4).

# **Algorithm 3** Formal computation of $(V_{\Re}^*(S_t))_{0 \le t \le m}$

240

241

242

245

```
procedure Curve(\Re = (R_k, \zeta_k)_{k \in \mathcal{X}} with \Re complete, path (S_t)_{1 \le t \le m} with S_t = \{i_1, \dots, i_t\})
             \mathcal{P}^0 \leftarrow \{(i,i) : 1 \le i \le n\}
 2:
                                                                                                                                the set of all atoms indices
             \mathcal{K}_0^- \leftarrow \{k \in \mathcal{K} : \zeta_k = 0\}
 3:
             \eta_k^0 \leftarrow 0 for all k \in \mathcal{K}
  4:
             for t = 1, \dots, m do
  5:
                    if i_t \in \bigcup_{k \in \mathcal{K}_{t-1}^-} R_k then \mathcal{P}^t \leftarrow \mathcal{P}^{t-1}
 6:
 7:
                          \begin{aligned} \mathcal{K}_t^- &\leftarrow \mathcal{K}_{t-1}^- \\ \eta_k^t &\leftarrow \eta_k^{t-1} \text{ for all } k \in \mathcal{K} \end{aligned}
  8:
 9:
10:
                           for h = 1, ..., h_{max}(t) do
11:
                                 \eta_{k^{(t,h)}}^t \leftarrow \eta_{k^{(t,h)}}^{t-1} + 1
12:
                                 if \eta_{k^{(t,h)}}^t < \zeta_k then
13:
14:
15:
                                 else
                                       h_t^f \leftarrow h
                                                                                                                                                             ⊳ final depth
16:
                                       \mathcal{P}^t \leftarrow \left(\mathcal{P}^{t-1} \setminus \{k \in \mathcal{P}^{t-1} : R_k \subseteq R_{k^{(t,h_t^f)}}\}\right) \cup \{k^{(t,h_t^f)}\}
17:
                                       \mathcal{K}_t^- \leftarrow \mathcal{K}_{t-1}^- \cup \{k^{(t,h_t^f)}\}
18:
                                        Break the loop
19:
                                 end if
20:
21:
                          end for
                          if the loop has been broken then
22:
                                 \eta_k^t \leftarrow \eta_k^{t-1} \text{ for all } k \in \mathcal{K} \text{ not visited during the loop, that is all } k \not \in \{k^{(t,h)}, 1 \leq h \leq t \}
23:
24:
                                 \mathcal{P}^t \leftarrow \mathcal{P}^{t-1}
25:
26:
                                 27:
      h_{\max}(t)
                           end if
28:
                    end if
29:
30:
             return \mathcal{P}^t, \eta_k^t for all t = 1, ..., m and k \in \mathcal{K}
31:
32: end procedure
```

The core idea of the algorithm is that, as we increase t and add new hypotheses in  $S_t$ , we inflate a counter  $\eta_k^t$  for each region  $R_k$ , by one if  $i_t \in R_k$  (line 12), by 0 if not (lines 23 and 27), but only until the counter reaches  $\zeta_k$  (line 13). After this point, the hypotheses in  $R_k$  don't contribute to  $V_{\mathfrak{R}}^*(S_t)$ , we keep track of those hypotheses with  $\mathcal{K}_t^-$  (line 6), so as soon as  $\eta_{k^{(t,h)}}^t = \zeta_k$  we update  $\mathcal{K}_t^-$  by adding  $k^{(t,h)}$  (line 18) to it and we update  $\mathcal{F}^t$  accordingly (line 17). We will see that  $V_{\mathfrak{R}}^*(S_t)$  is the sum of the  $\eta_k^t$  counters for  $k \in \mathcal{K}^1$ . Furthermore, the algorithm provides the partition  $\mathcal{F}^t \in \mathfrak{P}$  where the minimum in (12) is realized. We formalize all of that in the following Theorem. We first need a final

247 notation. Let

$$\mathcal{K}_t = \{k \in \mathcal{K} : \exists k' \in \mathcal{P}^t : R_{k'} \subseteq R_k\}.$$

The elements of  $\mathcal{K}_t$  index the regions of the forest that "are above" the regions of the current partition-realizing  $\mathcal{P}^t$ . In particular, we always have, for any  $t \in \mathbb{N}_m$ ,  $\mathcal{K}^1 \subseteq \mathcal{K}_t$  and  $\mathcal{P}^t \subseteq \mathcal{K}_t$ . We can also remark that the sequence  $(\mathcal{K}_t)_{0 \le t \le m}$  is non-increasing for the inclusion relation, and that  $\mathcal{K}_0 = \mathcal{K}$ .

Theorem 3.1 (Fast curve computation). Let any  $t \in \mathbb{N}_m$ . Then,  $\mathscr{P}^t \in \mathfrak{P}$ , and for all  $k \in \mathscr{K}_t$ , we have

$$V_{\mathfrak{R}}^{\star}(S_t \cap R_k) = \eta_k^t \tag{16}$$

253 and

$$V_{\mathfrak{R}}^{\star}(S_t \cap R_k) = \sum_{\substack{k' \in \mathscr{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_t \cap R_{k'}|. \tag{17}$$

254 Furthermore,

$$V_{\mathfrak{R}}^{\star}(S_t) = \sum_{k \in \mathscr{P}^t} \zeta_k \wedge |S_t \cap R_k| = \sum_{k \in \mathscr{K}^1} \eta_k^t.$$
 (18)

The first equality of Equation (18) confirms that the minimum in (12) is indeed realized on  $\mathscr{P}^t$ , and the last equality of the same Equation justifies the simpler Algorithm 4 to compute the curve on the nested path of selection sets (the  $V_t$  notation of Algorithm 4 is exactly the  $\sum_{k \in \mathscr{K}^1} \eta_k^t$  of Algorithm 3).

258 *Proof.* • Derivation of (18).

We first derive (18) from (16) and (17). First note that for all  $Q \in \mathfrak{P}$ ,

$$Q = \bigcup_{k \in \mathcal{K}^1} \{ k' \in Q : R_{k'} \subseteq R_k \}$$
 (19)

and the union is disjoint. From (12), let  $Q^* \in \mathfrak{P}$  such that  $V_{\mathfrak{R}}^*(S_t) = \sum_{k' \in Q^*} \zeta_{k'} \wedge |S_t \cap R_{k'}|$ . Then by (19),

$$V_{\mathfrak{R}}^{*}(S_{t}) = \sum_{k' \in \mathcal{Q}^{*}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}|$$

$$= \sum_{k \in \mathcal{K}^{1}} \sum_{\substack{k' \in \mathcal{Q}^{*} \\ R_{k'} \subseteq R_{k}}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}|$$

$$= \sum_{k \in \mathcal{K}^{1}} \sum_{\substack{k' \in \mathcal{Q}^{*} \\ R_{k'} \subseteq R_{k}}} \zeta_{k'} \wedge |S_{t} \cap (R_{k} \cap R_{k'})|$$

$$= \sum_{k \in \mathcal{K}^{1}} \sum_{\substack{k' \in \mathcal{Q}^{*} \\ R_{k'} \subseteq R_{k}}} \zeta_{k'} \wedge |(S_{t} \cap R_{k}) \cap R_{k'}|$$

$$\geq \sum_{k \in \mathcal{K}^{1}} V_{\mathfrak{R}}^{*}(S_{t} \cap R_{k}), \tag{21}$$

where the equality in (20) comes from the fact that if  $R_{k'} \nsubseteq R_k$ , then  $R_{k'} \cap R_k = \emptyset$ , that is,  $R_k \subseteq R_{k'}$  is impossible because  $k \in \mathcal{K}^1$ . Furthermore, (21) holds again by (12).

Because  $\mathcal{K}^1 \subseteq \mathcal{K}_t$ , by (17),  $V_{\mathfrak{R}}^*(S_t \cap R_k) = \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_t \cap R_{k'}|$  for all  $k \in \mathcal{K}^1$ . Then,

$$\sum_{k \in \mathcal{K}^1} V_{\mathfrak{R}}^*(S_t \cap R_k) = \sum_{k \in \mathcal{K}^1} \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_t \cap R_{k'}|$$

$$= \sum_{k \in \mathcal{P}^t} \zeta_k \wedge |S_t \cap R_k| \text{ by (19)}$$

$$\geq V_{\mathfrak{R}}^*(S_t) \text{ by (12)}.$$

So we proved that  $V_{\mathfrak{R}}^{\star}(S_t) = \sum_{k \in \mathscr{X}^1} \zeta_k \wedge |S_t \cap R_k| = \sum_{k \in \mathscr{K}^1} V_{\mathfrak{R}}^{\star}(S_t \cap R_k)$  and finally  $V_{\mathfrak{R}}^{\star}(S_t) = \sum_{k \in \mathscr{K}^1} V_{\mathfrak{R}}^{\star}(S_t \cap R_k) = \sum_{k \in \mathscr{K}^1} \eta_k^t$  by (16), again because  $\mathscr{K}^1 \subseteq \mathscr{K}_t$ . Every equality in (18) is proven.

• Proof of (16) and (17).

We show the remainder of the statements by strong recursion over t. We have  $\mathscr{P}^0 \in \mathfrak{P}$  by definition, and given that  $S_0 = \emptyset$  and  $\eta_k^0 = 0$  for all  $k \in \mathscr{K}$  (recall that  $\mathscr{K}_0 = \mathscr{K}$ ), everything is equal to 0 in (16) and (17).

So we let  $t \in \{0, ..., m-1\}$ , and assume that  $\mathcal{P}^{t'} \in \mathfrak{P}$  and that (16) and (17) hold for all  $t' \leq t$ .

In all the following,  $\bar{k}$  is the element of  $\mathcal{P}^t$  such that  $i_{t+1} \in R_{\bar{k}}$ . We will distinguish two cases: if  $i_{t+1} \in \bigcup_{k \in \mathcal{K}_t} R_k$  or not. First we show an inequality that will be used in both cases. We have, for all  $k \in \mathcal{K}_t$ ,

$$V_{\mathfrak{R}}^{\star}(S_{t+1} \cap R_k) \leq \sum_{\substack{k' \in \mathscr{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}|. \tag{22}$$

275 Indeed, by (12),

$$V_{\mathfrak{R}}^{\star}(S_{t+1} \cap R_k) \leq \sum_{k' \in \mathscr{P}^t} \zeta_{k'} \wedge |S_{t+1} \cap R_k \cap R_{k'}|.$$

For any  $k' \in \mathscr{P}^t$ , we have either  $R_{k'} \cap R_k = \emptyset$ , in which case  $|S_{t+1} \cap R_k \cap R_{k'}| = 0$ , either  $R_{k'} \subseteq R_k$ , in which case  $|S_{t+1} \cap R_k \cap R_{k'}| = |S_{t+1} \cap R_{k'}|$ , but  $R_k \subseteq R_{k'}$  is impossible. Indeed, by definition of  $\mathscr{K}_t$ , there exists  $\tilde{k} \in \mathscr{P}^t$  such that  $R_{\tilde{k}} \subseteq R_k$ , so  $R_k \subseteq R_{k'}$  would entail  $R_{\tilde{k}} \subseteq R_{k'}$  which is impossible since  $k', \tilde{k} \in \mathscr{P}^t \in \mathfrak{P}$  and so  $R_{\tilde{k}}$  are part of a partition of  $\mathbb{N}_m^*$ . This gives (22).

•• First case:  $i_{t+1} \in \bigcup_{k \in \mathcal{K}_t^-} R_k$ .

In this case,  $\mathscr{P}^{t+1} = \mathscr{P}^t \in \mathfrak{P}$  and  $\mathscr{K}_{t+1} = \mathscr{K}_t$ . For any  $k \in \mathscr{K}_{t+1}$  such that  $i_{t+1} \notin R_k$  (or, equivalently, such that  $S_{t+1} \cap R_k = S_t \cap R_k$ ),

$$\sum_{\substack{k' \in \mathcal{P}^{t+1} \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| = \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_t \cap R_{k'}|$$

$$= V_{\Re}^* (S_t \cap R_k) \text{ by (17)}$$

$$= \eta_k^t \text{ by (16)}$$

$$= \eta_k^{t+1}$$

because  $\eta_k^t = \eta_k^{t+1}$  for all  $k \in \mathcal{K}$ . Furthermore  $S_{t+1} \cap R_k = S_t \cap R_k$  so  $V_{\mathfrak{R}}^*(S_{t+1} \cap R_k) = V_{\mathfrak{R}}^*(S_t \cap R_k)$ . So everything is proved for such a k.

Now we let  $k \in \mathcal{K}_{t+1}$  such that  $i_{t+1} \in R_k$  or, equivalently, such that  $R_{\bar{k}} \subseteq R_k$ . We first need to show that  $\zeta_{\bar{k}} \leq |S_t \cap R_{\bar{k}}|$ , and for that we need to distinguish two subcases: if  $\bar{k}$  has been added to  $\mathcal{P}^t$  during a previous step of the algorithm, of if not.

••• First subcase:  $\bar{k}$  has never been added during the process of line 17.

Then  $\bar{k} \in \mathscr{P}^0$  and  $R_{\bar{k}}$  is an atom, so  $i_{t+1} \in \bigcup_{k' \in \mathscr{K}_t^-} R_{k'}$  implies that  $R_{\bar{k}} \subseteq \bigcup_{k' \in \mathscr{K}_t^-} R_{k'}$  (because of the forest structure). Let  $k'_{\max}$  such that

$$R_{k'_{\max}} = \max\{R_{k'} : k' \in \mathcal{K}_t^-, R_{\bar{k}} \subseteq R_{k'}\}$$

(this a maximum for the inclusion relation, and it is well defined thanks to the forest structure). By reductio ad absurdum we show that  $k'_{\max} = \bar{k}$ . If that wasn't the case, by the joint construction of  $\mathscr{P}^t$  and  $\mathscr{K}^-_t$  during the algorithm we would have  $k'_{\max} \in \mathscr{P}^t$  and a contradiction with the fact that  $\mathscr{P}^t \in \mathfrak{P}$ : we can't have both  $\bar{k} \in \mathscr{P}^t$  and  $k'_{\max} \in \mathscr{P}^t$  if they are distinct. So  $k'_{\max} = \bar{k}$ , so  $\bar{k} \in \mathscr{K}^-_t$ , but it cannot have been added to  $\mathscr{K}^-_t$  during a previous step of the algorithm, otherwise it would have been added to  $\mathscr{P}^t$ , too. Hence  $\bar{k} \in \mathscr{K}^-_0$  which means that  $\zeta_{\bar{k}} = 0$  and  $\zeta_{\bar{k}} = 0 \leq |S_t \cap R_{\bar{k}}|$ .

••• Second subcase:  $\bar{k}$  has been added to  $\mathscr{P}^t$  at a previous step.

Let  $t' \leq t$  be this step. This means that  $\bar{k} = k^{(t',h^f_{t'})}$  and that at that step  $\eta^{t'}_{\bar{k}} = \zeta_{\bar{k}}$ . Indeed, the if condition in line 13 failed so  $\eta^{t'}_{\bar{k}} \geq \zeta_{\bar{k}}$ , but for all t'' < t' we had  $\eta^{t''}_{\bar{k}} \leq \zeta_{\bar{k}}$  which implies equality. Also  $\bar{k} \in \mathscr{P}^{t'}$  so  $\bar{k} \in \mathscr{K}_{t'}$  so we can write

$$\zeta_{\bar{k}} = \eta_{\bar{k}}^{t'}$$

$$= V_{\mathfrak{R}}^{\star}(S_{t'} \cap R_{\bar{k}}) \text{ by (16)}$$

$$\leq |S_{t'} \cap R_{\bar{k}}|$$

$$\leq |S_t \cap R_{\bar{k}}|.$$

This concludes the two subcases dichotomy:  $\zeta_{\bar{k}} \leq |S_t \cap R_{\bar{k}}|$  and we can go back to our  $k \in \mathcal{K}_{t+1}$  such that  $i_{t+1} \in R_k$  and  $R_{\bar{k}} \subseteq R_k$ .

We write the following chain:

$$V_{\mathfrak{R}}^{*}(S_{t+1} \cap R_{k}) \leq \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k}}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| \text{ by (22) and } \mathscr{X}_{t+1} \subseteq \mathscr{K}_{t}$$

$$= \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ k' \neq k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| + \zeta_{\bar{k}} \wedge |S_{t+1} \cap R_{\bar{k}}|$$

$$= \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ k' \neq \bar{k}}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}| + \zeta_{\bar{k}} \wedge (|S_{t} \cap R_{\bar{k}}| + 1)$$

$$= \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ k' \neq \bar{k}}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}| + \zeta_{\bar{k}} \wedge |S_{t} \cap R_{\bar{k}}| \text{ because } \zeta_{\bar{k}} \leq |S_{t} \cap R_{\bar{k}}|$$

$$= \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ K' \neq \bar{k}}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}|$$

$$= V_{\mathfrak{R}}^{*}(S_{t} \cap R_{k}) \text{ by (17)}$$

$$= \eta_{k}^{t} \text{ by (16)}$$

$$= \eta_{k}^{t+1}.$$

But on the other hand,  $S_t \subseteq S_{t+1}$  and so (12) also gives  $V_{\mathfrak{R}}^*(S_t \cap R_k) \le V_{\mathfrak{R}}^*(S_{t+1} \cap R_k)$  and so in the end we have the desired outcome:

$$V_{\mathfrak{R}}^{*}(S_{t+1} \cap R_{k}) = \eta_{k}^{t+1} = \sum_{\substack{k' \in \mathcal{P}^{t+1} \\ R_{k'} \subseteq R_{k}}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}|,$$

- which concludes this first case.
- •• Second case:  $i_{t+1} \notin \bigcup_{k \in \mathcal{K}_t^-} R_k$ .
- First note that  $\mathscr{P}^{t+1} \in \mathfrak{P}$  whether it came form the adjustment in line 17 or it stayed equal to  $\mathscr{P}^t$ .
- Like in the first case, considering a  $k \in \mathcal{K}_{t+1} \subseteq \mathcal{K}_t$  such that  $i_{t+1} \notin R_k$  is not problematic, because in that case k is not visited at all by the algorithm at step  $t+1: \eta_k^{t+1} = \eta_k^t, \{k' \in \mathcal{P}^{t+1}: R_{k'} \subseteq R_k\} = \{k' \in \mathcal{P}^t: R_{k'} \subseteq R_k\}$ , and for all  $k' \in \mathcal{K}$  such that  $R_{k'} \subseteq R_k, S_{t+1} \cap R_{k'} = S_t \cap R_{k'}$ . Hence, from

$$V_{\mathfrak{R}}^{\star}(S_t \cap R_k) = \eta_k^t = \sum_{\substack{k' \in \mathscr{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}|,$$

312 we directly have

$$V_{\mathfrak{R}}^{*}(S_{t+1} \cap R_{k}) = \eta_{k}^{t+1} = \sum_{\substack{k' \in \mathcal{P}^{t+1} \\ R_{t,i} \subset R_{t}}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}|.$$

First note that for all  $k \in \mathcal{K}_{t+1}$  such that  $i_{t+1} \in R_k$ ,

$$\eta_k^{t+1} = \eta_k^t + 1 = V_{\Re}^*(S_t \cap R_k) + 1 = \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_t \cap R_{k'}| + 1$$

by construction, by (16) and by (17). Indeed, such a k is equal to a  $k^{(t+1,h)}$  with  $h \le h_{max}(t+1)$ , and even  $h \le h_{t+1}^f$  if the latter exists.

Also, similarly to the first case, for all  $k \in \mathcal{K}_{t+1}$  such that  $i_{t+1} \in R_k$  (recall that this is equivalent to  $R_{\bar{k}} \subseteq R_k$ ), we can write:

$$V_{\Re}^{\star}(S_{t+1} \cap R_{k}) \leq \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k}}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| \text{ by (22) and } \mathscr{X}_{t+1} \subseteq \mathscr{K}_{t}$$

$$= \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ R' \neq \bar{k}}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| + \zeta_{\bar{k}} \wedge |S_{t+1} \cap R_{\bar{k}}|$$

$$= \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ k' \neq \bar{k}}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}| + \zeta_{\bar{k}} \wedge (|S_{t} \cap R_{\bar{k}}| + 1)$$

$$\leq \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ k' \neq \bar{k}}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}| + \zeta_{\bar{k}} \wedge |S_{t} \cap R_{\bar{k}}| + 1$$

$$= \sum_{\substack{k' \in \mathscr{P}^{t} \\ R_{k'} \subseteq R_{k} \\ k' \neq \bar{k}}} \zeta_{k'} \wedge |S_{t} \cap R_{k'}| + 1$$

$$= V_{\Re}^{\star}(S_{t} \cap R_{k}) + 1 \text{ by (17)}. \tag{23}$$

Note that by the joint construction of  $\mathcal{K}_t^-$  and  $\mathcal{S}^t$  on lines 17 and 18, the fact that  $i_{t+1} \notin \bigcup_{k \in \mathcal{K}_t^-} R_k$  implies that  $\bar{k}$  is the index of an atom, so actually  $h_{\max}(t+1) = \phi(\bar{k})$ ,  $\bar{k} = k^{(t+1,\phi(\bar{k}))}$  and the  $R_k$ ,  $k \in \mathcal{K}_t$ , such that  $R_{\bar{k}} \subseteq R_k$  are nested and are exactly indexed by the  $k^{(t+1,h)}$ ,  $1 \le h \le \phi(\bar{k})$ . We now prove that for all of them,  $V_{\mathfrak{R}}^*(S_{t+1} \cap R_k) \ge V_{\mathfrak{R}}^*(S_t \cap R_k) + 1$ , which will be true in particular for the ones that are in  $\mathcal{K}_{t+1}$ , given that  $\mathcal{K}_{t+1} \subseteq \mathcal{K}_t$ . We do that by constructing some sets  $A_h$  with good properties with a descending recursion on h, starting from  $\phi(\bar{k})$ . We only give the first two steps of the construction, because every other step is exactly the same as the second one, which contains the recursive arguments. We go back to the real definition of  $V_{\mathfrak{R}}^*$  to do so, for any  $S \subseteq \mathbb{N}_m$ :

$$V_{\mathfrak{R}}^{*}(S) = \max_{\substack{A \subseteq \mathbb{N}_{m} \\ \forall k' \in \mathcal{K}, |A \cap R_{k'}| \le \zeta_{k'}}} |A \cap S| = \max_{\substack{A \subseteq S \\ \forall k' \in \mathcal{K}, |A \cap R_{k'}| \le \zeta_{k'}}} |A|. \tag{24}$$

By (24), we have that  $V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}) = |A_{\phi(\bar{k})}|$  for a given  $A_{\phi(\bar{k})} \subseteq S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}$  and such that  $|A_{\phi(\bar{k})} \cap R_{k'}| \leq \zeta_{k'}$  for all  $k' \in \mathcal{K}$ . Now for the second set, we construct  $A_{\phi(\bar{k})-1}$ . Note that  $V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}) = |B|$  for some  $B \subseteq S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}$  and such that  $|B \cap R_{k'}| \leq \zeta_{k'}$  for all  $k' \in \mathcal{K}$ . By reductio ad absurdum, if there are strictly less than  $V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}) - V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}) = |B| - |A_{\phi(\bar{k})}|$  elements in  $S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}} \setminus S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}$ , then  $|B| + |S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}| - |S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}| > |A_{\phi(\bar{k})}| = V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k}))}})$ . Given that  $B \cup (S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}) \subseteq S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}$ , this entails  $|B \cap S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}| = |B| + |S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}| - |B \cup (S_t \cap R_{k^{(t+1,\phi(\bar{k}))}})| > V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k}))}})$  which contradicts the maximality of  $A_{\phi(\bar{k})}$  in (24).

So we construct  $A_{\phi(\bar{k})-1}$  by taking the disjoint union of  $A_{\phi(\bar{k})}$  and  $V_{\Re}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}) - V_{\Re}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k}))}})$  elements of  $S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}} \setminus S_t \cap R_{k^{(t+1,\phi(\bar{k}))}}$ . We now establish the properties of  $A_{\phi(\bar{k})-1}$ . First,  $A_{\phi(\bar{k})-1} \subseteq S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}$ , and  $|A_{\phi(\bar{k})-1}| = V_{\Re}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}})$ . For all  $k' \in \mathscr{K}$  such that  $R_{k^{(t+1,\phi(\bar{k})-1)}} \cap R_{k'} = \emptyset$ , we have  $|A_{\phi(\bar{k})-1} \cap R_{k'}| = 0 \le \zeta_k'$ . Furthermore,

$$|A_{\phi(\bar{k})-1} \cap R_{k^{(t+1,\phi(\bar{k}))}}| = |A_{\phi(\bar{k})} \cap R_{k^{(t+1,\phi(\bar{k}))}}|$$

$$\leq \zeta_{k(t+1,\phi(\bar{k}))}$$

by construction of  $A_{\phi(\bar{k})}$ . Finally, for all k' such that  $R_{k^{(t+1,\phi(\bar{k})-1)}} \subseteq R_{k'}$ ,  $|A_{\phi(\bar{k})-1} \cap R_{k'}| = |A_{\phi(\bar{k})-1}| = V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}) = |B|$  with the previously defined B, in particular  $|B \cap R_{k'}| \leq \zeta_{k'}$ , but given that  $B \subseteq S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}$ ,  $|B \cap R_{k'}| = |B|$ . Wrapping all those equalities, it comes that  $|A_{\phi(\bar{k})-1} \cap R_{k'}| \leq \zeta_{k'}$ . In the end,  $|A_{\phi(\bar{k})-1} \cap R_{k'}| \leq \zeta_{k'}$  for all  $k' \in \mathcal{K}$ , so  $A_{\phi(\bar{k})-1}$  realizes the maximum in (24) for  $S_t \cap R_{k^{(t+1,\phi(\bar{k})-1)}}$ .

By applying exactly the same method, we recursively construct a non-increasing sequence  $A_{\phi(\bar{k})} \subseteq \cdots \subseteq A_1$  such that for all  $\ell \in \{1, \dots, \phi(\bar{k})\}$  and  $k' \in \mathcal{K}$ ,  $A_{\ell} \subseteq S_t \cap R_{k^{(t+1,\ell)}}$ ,  $V_{\mathfrak{R}}^*(S_t \cap R_{k^{(t+1,\ell)}}) = |A_{\ell}|$ , and  $|A_{\ell} \cap R_{k'}| \leq \zeta_{k'}$ . Furthermore for  $\ell' > \ell$ ,  $A_{\ell} \setminus A_{\ell'} \subseteq S_t \cap R_{k^{(t+1,\ell)}} \setminus S_t \cap R_{k^{(t+1,\ell)}}$ . Also note that the fact that  $i_{t+1} \notin \bigcup_{k \in \mathcal{K}_t^-} R_k$  implies that  $\eta_{k^{(t+1,\ell)}}^t < \zeta_{k^{(t+1,\ell)}}$  for all  $\ell \in \{1, \dots, \phi(\bar{k})\}$ . So by (16),  $|A_{\ell}| < \zeta_{k^{(t+1,\ell)}}$ .

Let, for any  $\ell \in \{1, \dots, \phi(\bar{k})\}$ ,  $\widetilde{A}_{\ell} = A_{\ell} \cup \{i_{t+1}\}$ . Given that  $A_{\ell} \subseteq S_t \cap R_{k^{(t+1,\ell)}}$  and that  $i_{t+1} \in S_{t+1} \setminus S_t$ ,  $\widetilde{A}_{\ell} \subseteq S_{t+1} \cap R_{k^{(t+1,\ell)}}$ ,  $|\widetilde{A}_{\ell}| = |A_{\ell}| + 1$ , and for all  $\ell' \in \{1, \dots, \phi(\bar{k})\}$ ,  $|\widetilde{A}_{\ell} \cap R_{k^{(t+1,\ell)}}| = |A_{\ell} \cap R_{k^{(t+1,\ell)}}| + 1$ . Note that if, furthermore,  $\ell \geq \ell'$ , then  $A_{\ell} \subseteq A_{\ell'}$ , so

$$\begin{split} |\widetilde{A}_{\ell} \cap R_{k^{(t+1,\ell')}}| &= |A_{\ell} \cap R_{k^{(t+1,\ell')}}| + 1 \\ &\leq |A_{\ell'} \cap R_{k^{(t+1,\ell')}}| + 1 \\ &= |A_{\ell'}| + 1 \\ &< \zeta_{k^{(t+1,\ell')}} + 1. \end{split}$$

On the contrary, if  $\ell < \ell'$ , we write that

$$\begin{split} |\widetilde{A}_{\ell} \cap R_{k^{(t+1,\ell')}}| &= |A_{\ell} \cap R_{k^{(t+1,\ell')}}| + 1 \\ &= |(A_{\ell} \setminus A_{\ell'}) \cap R_{k^{(t+1,\ell')}}| + |A_{\ell'} \cap R_{k^{(t+1,\ell')}}| + 1 \\ &< 0 + \zeta_{k^{(t+1,\ell')}} + 1, \end{split}$$

because  $A_{\ell} \setminus A_{\ell'} \subseteq R_{k^{(t+1,\ell')}} \setminus R_{k^{(t+1,\ell')}}$  hence  $(A_{\ell} \setminus A_{\ell'}) \cap R_{k^{(t+1,\ell')}} = \emptyset$ . In both cases,  $|\widetilde{A}_{\ell} \cap R_{k^{(t+1,\ell')}}| < \zeta_{k^{(t+1,\ell')}} + 1$  so  $|\widetilde{A}_{\ell} \cap R_{k^{(t+1,\ell')}}| \le \zeta_{k^{(t+1,\ell')}}$ . Additionally, for all  $k' \in \mathcal{K}$  such that  $i_{t+1} \notin R_{k'}$ ,  $|\widetilde{A}_{\ell} \cap R_{k'}| = |A_{\ell} \cap R_{k'}| \le \zeta_{k'}$ .

In the end,  $|\widetilde{A}_{\ell} \cap R_{k'}| \leq \zeta_{k'}$  for all  $k' \in \mathcal{K}$ , so

$$\begin{split} V_{\mathfrak{R}}^{\star}(S_{t+1} \cap R_{k^{(t+1,\ell)}}) &\geq |\widetilde{A}_{\ell}| \text{ by (24)} \\ &= |A_{\ell}| + 1 \\ &= V_{\mathfrak{R}}^{\star}(S_{t} \cap R_{k^{(t+1,\ell)}}) + 1. \end{split}$$

So, as we wanted,  $V_{\mathfrak{R}}^{\star}(S_{t+1} \cap R_k) \geq V_{\mathfrak{R}}^{\star}(S_t \cap R_k) + 1$  for all  $k \in \mathcal{K}_t$  such that  $i_{t+1} \in R_k$  and so for all such k that are in  $\mathcal{K}_{t+1}$ . So every inequality in (23) becomes an equality and we have proven that

$$V_{\mathfrak{R}}^*(S_{t+1} \cap R_k) = V_{\mathfrak{R}}^*(S_t \cap R_k) + 1 = \eta_k^t + 1 = \eta_k^{t+1},$$

that is, (16) is true at t + 1. Looking at the first line of (23), we also proved that

$$V_{\mathfrak{R}}^{\star}(S_{t+1} \cap R_k) = \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}|. \tag{25}$$

The only thing left to prove is that (25) is also true with  $\mathcal{P}^{t+1}$  instead of  $\mathcal{P}^t$ , that is, (17) also holds at t+1. If  $h_{t+1}^f$  does not exist, meaning that we didn't break the loop,  $\mathcal{P}^{t+1} = \mathcal{P}^t$  so there is nothing to prove.

Now assume that  $h_{t+1}^f$  exists. So

$$\mathscr{P}^{t+1} = \left( \mathscr{P}^t \setminus \{k \in \mathscr{P}^t, R_k \subseteq R_{L^{(t+1,h_{t+1}^f)}}\} \right) \cup \{k^{(t+1,h_{t+1}^f)}\}.$$

Note that for all  $k \in \mathcal{K}_{t+1}$  such that  $i_{t+1} \in R_k$ , we necessarily have  $R_{k^{(t+1,h_{t+1}^f)}} \subseteq R_k$ , because  $k^{(t+1,h_{t+1}^f)} \in \mathcal{P}^{t+1}$ . Also note that for  $k' \in \mathcal{P}^t$ , we either have  $R_{k'} \cap R_{k^{(t+1,h_{t+1}^f)}} = \emptyset$  or  $R_{k'} \subseteq R_{k^{(t+1,h_{t+1}^f)}}$ , by the operation made in line 17. So we can split

$$\sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| = \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \cap R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| + \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}|$$

364 and

$$\begin{split} \sum_{\substack{k' \in \mathcal{P}^{t+1} \\ R_{k'} \subseteq R_k}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| &= \sum_{\substack{k' \in \mathcal{P}^{t+1} \\ R_{k'} \cap R_{k^{(t+1,h_{t+1}^f)}} = \emptyset}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| + \zeta_{k^{(t+1,h_{t+1}^f)}} \wedge |S_{t+1} \cap R_{k^{(t+1,h_{t+1}^f)}}| \\ &= \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \cap R_{k^{(t+1,h_{t+1}^f)}} = \emptyset}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| + \zeta_{k^{(t+1,h_{t+1}^f)}} \wedge |S_{t+1} \cap R_{k^{(t+1,h_{t+1}^f)}}|. \end{split}$$

So, we just need to prove that

$$\sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_{k'}(t+1,h_{t+1}^f)}} \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| = \zeta_{k^{(t+1,h_{t+1}^f)}} \wedge |S_{t+1} \cap R_{k^{(t+1,h_{t+1}^f)}}|.$$

Interestingly, this does not depend on k anymore. By (25), the left-hand side is equal to  $V_{\mathfrak{R}}^{\star}(S_{t+1} \cap R_{k^{(t+1,h_{t+1}^f)}})$ . Because we are breaking the loop at step  $h_{t+1}^f$ ,  $\eta_{k^{(t+1,h_{t+1}^f)}}^{t+1} = \zeta_{k^{(t+1,h_{t+1}^f)}}$ . Finally, because (16) holds at t+1,  $\eta_{k^{(t+1,h_{t+1}^f)}}^{t+1} = V_{\mathfrak{R}}^{\star}(S_{t+1} \cap R_{k^{(t+1,h_{t+1}^f)}})$ . Wrapping all this assertions:

$$\begin{split} \sum_{\substack{k' \in \mathcal{P}^t \\ R_{k'} \subseteq R_{\underline{k}^{(t+1,h_{t+1}^f)}}} & \zeta_{k'} \wedge |S_{t+1} \cap R_{k'}| = V_{\mathfrak{R}}^*(S_{t+1} \cap R_{\underline{k}^{(t+1,h_{t+1}^f)}}) \\ &= V_{\mathfrak{R}}^*(S_{t+1} \cap R_{\underline{k}^{(t+1,h_{t+1}^f)}}) \wedge |S_{t+1} \cap R_{\underline{k}^{(t+1,h_{t+1}^f)}}| \\ &= \eta_{\underline{k}^{(t+1,h_{t+1}^f)}}^{t+1} \wedge |S_{t+1} \cap R_{\underline{k}^{(t+1,h_{t+1}^f)}}| \\ &= \zeta_{\underline{k}^{(t+1,h_{t+1}^f)}} \wedge |S_{t+1} \cap R_{\underline{k}^{(t+1,h_{t+1}^f)}}|, \end{split}$$

which achieves the second case and so the proof.

370

We deduce from the proof the following light corollary, that is useful for the implementation, because it makes it useless to compute  $\mathcal{K}^1$ . It justifies the line 19 of Algorithm 4.

Corollary 3.1 (Easy computation). For  $t \in \{0, ..., m-1\}$ ,  $V_{\Re}^*(S_{t+1}) = V_{\Re}^*(S_t)$  if  $i_{t+1} \in \bigcup_{k \in \mathcal{K}_t^-} R_k$ , and  $V_{\Re}^*(S_{t+1}) = V_{\Re}^*(S_t) + 1$  if not.

Finally, we present Algorithm 4 , the alternative version of Algorithm 3 , written with practical implementation in mind rather than formalism of notation, and using Corollary 3.1. It is easy to see that each step t has a complexity in  $O(|\mathcal{K}|)$  hence the total complexity is in  $O(m|\mathcal{K}|)$ . This is because, if the regions are carefully stocked in memory, especially if their bounds (in terms of hypothesis index) are stocked, then finding  $k^{(t,h)}$  has a complexity in  $O(|\mathcal{K}^h|)$  and checking if  $i_t \in \bigcup_{k \in \mathcal{K}_{t-1}^-} R_k$  has a complexity in  $O(|\mathcal{K}|)$ .

# 4 Implementation

All algorithms discussed in this manuscript are already implemented in the R (R Core Team, 2020) pack-382 age sanssouci (Neuvial et al., 2024) which is available on GitHub (see the References for the link) and 383 is dedicated to the computation of confidence bounds for the number of false positives. It also hosts 384 the implementation of the methods described in Blanchard et al. (2020). Algorithm 1 is implemented 385 as the V. star function, Algorithm 2 is implemented as the pruning function, and Algorithm 4 is im-386 plemented as the curve.V.star.forest.fast function (whereas the curve.V.star.forest.naive 387 function just repeatedly calls V. star). Note that the pruning function has a delete.gaps option 388 that speeds up the computation even more by removing unnecessary gaps introduced in the data 389 structure by the pruning operation, those gaps being due to the specific structure that is used to 390 store the information of  $\mathcal{K}$ .

The functions dyadic.from.leaf\_list, dyadic.from.window.size, and dyadic.from.height return the appropriate data structure to represent a  $\mathcal{K}$  that can be described as a dyadic tree, based on some entry parameters that can be inferred from the names of the functions. The completion of a

# **Algorithm 4** Practical computation of $(V_{\Re}^*(S_t))_{0 \le t \le m}$

```
1: procedure Curve(\Re = (R_k, \zeta_k)_{k \in \mathcal{X}} with \Re complete, path (S_t)_{1 \le t \le m} with S_t = \{i_1, ..., i_t\})
 2:
             \mathcal{K}^- \leftarrow \{k \in \mathcal{K} : \zeta_k = 0\}
 3:
             \eta_k \leftarrow 0 \text{ for all } k \in \mathcal{K}
  4:
             for t = 1, ..., m do
  5:
                   if i_t \in \bigcup_{k \in \mathcal{K}^-} R_k then
 6:
                          V_t \leftarrow V_{t-1}
 7:
                   else
 8:
                          for h = 1, ..., h_{\max}(t) do find k^{(t,h)} \in \mathcal{K}^h such that i_t \in R_{k^{(t,h)}}
10:
                                 \eta_{k(t,h)} \leftarrow \eta_{k(t,h)} + 1
11:
                                 if \eta_{k^{(t,h)}} < \zeta_k then
12:
                                       pass
13:
14:
                                       \mathcal{K}^- \leftarrow \mathcal{K}^- \cup \{k^{(t,h)}\}
15:
                                       break the loop
16:
                                 end if
17:
                          end for
18:
                          V_t \leftarrow V_{t-1} + 1
19:
20:
                   end if
             end for
21:
22:
             return (V_t)_{1 \le t \le m}
23: end procedure
```

forest structure, mentioned in Section 2.3, is done by the forest.completion function. Finally, the  $\zeta_k$  are computed as in Durand et al. (2020) by the zetas.tree function with method=zeta.DKWM.

# **5 Numerical experiments**

In this Section, we present some numerical experiments aiming to demonstrate the impact of the pruning of Algorithm 2 (with and without the optimization of the delete.gaps option mentioned in Section 4) and of the fast Algorithm 4, in terms of computation time, compared to the only previously available method to compute a curve of confidence bounds. As mentioned in Section 2.3 and Section 4, this naive method simply consisted in a for loop repeatedly applying Algorithm 1.

#### 6 Conclusion

# 7 Acknowledments

This work has been supported by ANR-20-IDEES-0002 (PIA), ANR-19-CHIA-0021 (BISCOTTE), ANR-23-CE40-0018 (BACKUP) and ANR-21-CE23-0035 (ASCAI).

#### References

Yoav Benjamini and Yosef Hochberg. Controlling the false discovery rate: a practical and powerful
 approach to multiple testing. J. Roy. Statist. Soc. Ser. B, 57(1):289–300, 1995. ISSN 0035-9246. URL
 https://www.jstor.org/stable/2346101.

- Alexandre Blain, Bertrand Thirion, and Pierre Neuvial. Notip: Non-parametric True Discovery
  Proportion control for brain imaging. *Neuroimage*, 260, October 2022. URL https://doi.org/10.1016/j.neuroimage.2022.119492.
- Gilles Blanchard, Pierre Neuvial, and Etienne Roquain. Post hoc confidence bounds on false positives
   using reference families. *Ann. Statist.*, 48(3):1281–1303, 2020. ISSN 0090-5364. doi: 10.1214/19-AOS1847. URL https://doi.org/10.1214/19-AOS1847.
- Małgorzata Bogdan, Ewout van den Berg, Chiara Sabatti, Weijie Su, and Emmanuel J. Candès. SLOPE—
   adaptive variable selection via convex optimization. *Ann. Appl. Stat.*, 9(3):1103–1140, 2015. ISSN
   1932-6157,1941-7330. doi: 10.1214/15-AOAS842. URL https://doi.org/10.1214/15-AOAS842.
- Guillermo Durand, Gilles Blanchard, Pierre Neuvial, and Etienne Roquain. Post hoc false positive control for structured hypotheses. *Scand. J. Stat.*, 47(4):1114–1148, 2020. ISSN 0303-6898. doi: 10.1111/sjos.12453. URL https://doi.org/10.1111/sjos.12453.
- Christopher R. Genovese and Larry Wasserman. Exceedance control of the false discovery proportion. *J. Amer. Statist. Assoc.*, 101(476):1408–1417, 2006. ISSN 0162-1459. doi: 10.1198/016214506000000339.

  URL https://doi.org/10.1198/016214506000000339.
- Jelle J. Goeman and Aldo Solari. Multiple testing for exploratory research. *Statist. Sci.*, 26(4):584–597, 2011. ISSN 0883-4237. doi: 10.1214/11-STS356. URL https://doi.org/10.1214/11-STS356.
- Ruth Marcus, Eric Peritz, and K. R. Gabriel. On closed testing procedures with special reference to ordered analysis of variance. *Biometrika*, 63(3):655–660, 1976. ISSN 0006-3444. doi: 10.1093/biomet/63.3.655. URL https://doi.org/10.1093/biomet/63.3.655.
- Rosa J. Meijer, Thijmen J. P. Krebs, and Jelle J. Goeman. A region-based multiple testing method for hypotheses ordered in space or time. *Stat. Appl. Genet. Mol. Biol.*, 14(1):1–19, 2015. ISSN 2194-6302. doi: 10.1515/sagmb-2013-0075. URL https://doi.org/10.1515/sagmb-2013-0075.
- Nicolai Meinshausen. False discovery control for multiple tests of association under general dependence. Scand. J. Statist., 33(2):227–237, 2006. ISSN 0303-6898. doi: 10.1111/j.1467-9469.2005.00488.x.
   URL https://doi.org/10.1111/j.1467-9469.2005.00488.x.
- Pierre Neuvial, Gilles Blanchard, Guillermo Durand, Nicolas Enjalbert-Courrech, and Etienne Roquain.
   sanssouci: Post Hoc Multiple Testing Inference, 2024. URL https://sanssouci-org.github.io/sanssouci.
   R package version 0.13.0.
- R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2020. URL https://www.R-project.org/.
- Anna Vesely, Livio Finos, and Jelle J. Goeman. Permutation-based true discovery guarantee by sum tests. J. R. Stat. Soc. Ser. B. Stat. Methodol., 85(3):664–683, 2023. ISSN 1369-7412,1467-9868. doi: 10.1093/jrsssb/qkad019. URL https://doi.org/10.1093/jrsssb/qkad019.

#### Session information

445

```
R version 4.4.1 (2024-06-14)

Platform: x86_64-pc-linux-gnu

Running under: Ubuntu 22.04.5 LTS

Matrix products: default

BLAS: /usr/lib/x86_64-linux-gnu/blas/libblas.so.3.10.0

LAPACK: /usr/lib/x86_64-linux-gnu/lapack/liblapack.so.3.10.0
```

```
453
   locale:
    [1] LC_CTYPE=C.UTF-8
                                LC_NUMERIC=C
                                                        LC_TIME=C.UTF-8
    [4] LC_COLLATE=C.UTF-8
                                LC_MONETARY=C.UTF-8
                                                        LC_MESSAGES=C.UTF-8
456
    [7] LC_PAPER=C.UTF-8
                                LC_NAME=C
                                                        LC_ADDRESS=C
457
   [10] LC_TELEPHONE=C
                                LC_MEASUREMENT=C.UTF-8 LC_IDENTIFICATION=C
458
459
   time zone: Etc/UTC
460
   tzcode source: system (glibc)
   attached base packages:
463
                 graphics grDevices datasets utils
   [1] stats
                                                           methods
                                                                      base
464
   loaded via a namespace (and not attached):
                                                                 htmltools_0.5.8.1
    [1] compiler_4.4.1
                           fastmap_1.1.1
                                              cli_3.6.2
    [5] tools_4.4.1
                           yaml_2.3.8
                                              rmarkdown_2.26
                                                                 knitr_1.46
    [9] jsonlite_1.8.8
                           xfun_0.43
                                              digest_0.6.35
                                                                 rlang_1.1.3
   [13] renv_1.0.7
                           evaluate_0.23
```