

Instant-by-instant and simultaneous confidence prediction bands

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Abstract

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1 Introduction

[Here we are going to insert the reason why we do all of these]

Izbicki, Shimizu, and Stern (2019) proposed two methods for building prediction bands: CDist-split and CD-split based on split conformal prediction (Vovk, Gammerman, and Shafer, 2005). The prediction sets forming CDist-split bands are intervals whereas those forming CD-split ones are (estimated) density level sets which can take any form depending the shape of the conditional probability density function estimate (for instance a union of two intervals if the density is bimodal).

Izbicki, Shimizu, and Stern (2022) proposed yet another method for building prediction bands : HPD-split. The prediction sets forming HPD-split bands are also (estimated) density level sets. What differs from CD-split is that the chosen level varies with the input value, whereas for CD-split, the level is the same for every input value. In our context, our instant-by-instant prediction bands are index by the instant. Since for each instant, the probability distribution is supported on a discrete finite set, full conformal (no splitting) versions of CDist-split and CD-split are proposed.

Diquigiovanni, Fontana, and Vantini (2021) proposed a method for building prediction bands for functional data based on split conformal prediction (Vovk, Gammerman, and Shafer, 2005). This prediction band ensure control of coverage of the (random) function at every instant simultaneously. In contrast to their functions which are indexed by a continuous interval of instants, our curves are indexed by a finite discrete set of instants. **[TODO Davidson: This is a little weak]** In contrast to their bands, our γ -simultaneous bounds ensure control of coverage of the (random) curve only for a specified (supposed to be large) proportion of instants.

Section 2 discusses instant-by-instant prediction bands based on full conformal prediction (Vovk, Gammerman, and Shafer, 2005) version of CD-split, CDist-split in our context, along with one based on split conformal prediction of CDist-split.

Section 3 discusses γ -simultaneous prediction bands based on the previously mentioned instant-by-instant prediction bands.

2 Instant-by-Instant prediction band

3 Simultaneous prediction band

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Appendix

Definition 1. Let K the size of the fleet and T the size of the time grid be non-zero integers. Let a cumulative event number evolution curve $\xi = (\xi_1, \dots, \xi_T)$ be a random vector where for every $\tau \in \{1, \dots, T\}$, ξ_τ is a $\{1, \dots, K\}$ -valued random variable. Let a band $B = (B_1, \dots, B_T)$ be such that for every $\tau \in \{1, \dots, T\}$, $\hat{B}_{\alpha;\tau} \subseteq \{1, \dots, K\}$.

Definition 2 (Instant-by-instant coverage). Let $\alpha \in (0, 1)$. A band B controls the instant-by-instant coverage of the curve ξ at a control level α if

$$\forall \tau \in \{1, \dots, T\}, \quad \mathbb{P} \left[\xi_\tau \in \hat{B}_{\alpha;\tau} \right] \geq 1 - \alpha.$$

Definition 3 (γ -Simultaneous coverage). Let $\alpha \in (0, 1)$ and $\gamma \in [0, 1]$. A band B controls the γ -simultaneous coverage of the curve ξ at a control level α if

$$\mathbb{P} \left[\frac{\text{Card} \left(\left\{ \tau \in \{1, \dots, T\} : \xi_\tau \in \hat{B}_{\alpha;\tau} \right\} \right)}{T} \geq 1 - \gamma \right] \geq 1 - \alpha.$$

Proposition 1 (Instant-by-instant prediction band, MD-full). Let ξ_1, \dots, ξ_n be n independent copies of ξ . For any control level $\alpha \in [0, 1]$, the band $\hat{B}_{\alpha}^{\text{MD-full}}$ defined as, for every $\tau \in \{1, \dots, T\}$

$$\hat{B}_{\alpha;\tau}^{\text{MD-full}} := \left\{ k \in \{1, \dots, K\} : \hat{p}_\tau(k) \geq \hat{\ell}_{\alpha;\tau} - \frac{1}{n} \right\} \quad (1)$$

ensures control of the instant-by-instant coverage of ξ at a control level α , where the marginal empirical probability density function \hat{p}_τ is defined in Equation (Eq. (2)) and the threshold $\hat{\ell}_{\alpha;\tau}$ in Equation (Eq. (3)).

Proof of Proposition 1. Let $\alpha \in [0, 1]$ and $\tau \in \{1, \dots, T\}$. Following Lei, Robins, and Wasserman (2013), a full conformal prediction $\hat{C}_{\alpha;\tau}$ region is built from the observations $\xi_{1;\tau}, \dots, \xi_{n;\tau}$ for ξ_τ as follows

$$\hat{C}_{\alpha;\tau} = \{k \in \{1, \dots, K\} : \hat{\pi}_\tau(k) > \alpha\}$$

where for every $k \in \{1, \dots, K\}$

$$\hat{\pi}_\tau(k) := \frac{1 + \sum_{i=1}^n \mathbb{1} \{ \hat{p}_\tau^k(\xi_{i;\tau}) \leq \hat{p}_\tau^k(k) \}}{n + 1}$$

where for every $l \in \{1, \dots, K\}$

$$\hat{p}_\tau^k(l) = \frac{n}{n+1} \hat{p}_\tau(l) + \frac{1}{n+1} \mathbb{1} \{k = l\},$$

and the empirical marginal probability density function is given by

$$\hat{p}_\tau(l) = \frac{1}{n} \sum_{i=1}^n \mathbb{1} \{ \xi_{i;\tau} = l \} \quad (2)$$

Since $\xi_{1;\tau}, \dots, \xi_{n;\tau}$ are i.i.d. copies of ξ_τ , $\hat{C}_{\alpha;\tau}$ is a confidence prediction region (Vovk, Gamerman, and Shafer, 2005)

$$\mathbb{P} \left[\xi_\tau \in \hat{C}_{\alpha;\tau} \right] \geq 1 - \alpha.$$

Let us now provide an explicit expression of this region.

$$\begin{aligned}
k \in \hat{C}_{\alpha;\tau} &\iff \hat{\pi}_\tau(k) > \alpha \\
&\iff \frac{1 + \sum_{i=1}^n \mathbb{1} \left\{ \hat{p}_\tau^k(\xi_{i;\tau}) \leq \hat{p}_\tau^k(k) \right\}}{n+1} > \alpha \\
&\iff \frac{1}{n} \sum_{i=1}^n \mathbb{1} \left\{ \hat{p}_\tau^k(\xi_{i;\tau}) > \hat{p}_\tau^k(k) \right\} < (1-\alpha) \left(1 + \frac{1}{n} \right).
\end{aligned}$$

Let us consider the term on the l.h.s.

$$\begin{aligned}
&\frac{1}{n} \sum_{i=1}^n \mathbb{1} \left\{ \hat{p}_\tau^k(\xi_{i;\tau}) > \hat{p}_\tau^k(k) \right\} \\
&= \frac{1}{n} \sum_{i=1}^n \sum_{l=1}^K \mathbb{1} \{l = \xi_{i;\tau}\} \mathbb{1} \left\{ \hat{p}_\tau^k(\xi_{i;\tau}) > \hat{p}_\tau^k(k) \right\} \\
&= \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{p}_\tau^k(l) > \hat{p}_\tau^k(k) \right\} \\
&= \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \frac{n}{n+1} \hat{p}_\tau(l) + \frac{1}{n+1} \mathbb{1} \{k = l\} > \frac{n}{n+1} \hat{p}_\tau(k) + \frac{1}{n+1} \right\} \\
&= \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{p}_\tau(l) + \frac{1}{n} \mathbb{1} \{k = l\} > \hat{p}_\tau(k) + \frac{1}{n} \right\} \\
&= \hat{p}_\tau(k) \mathbb{1} \left\{ \hat{p}_\tau(k) + \frac{1}{n} > \hat{p}_\tau(k) + \frac{1}{n} \right\} + \sum_{l=1, l \neq k}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{p}_\tau(l) > \hat{p}_\tau(k) + \frac{1}{n} \right\} \\
&= \hat{p}_\tau(k) \mathbb{1} \left\{ \hat{p}_\tau(k) > \hat{p}_\tau(k) + \frac{1}{n} \right\} + \sum_{l=1, l \neq k}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{p}_\tau(l) > \hat{p}_\tau(k) + \frac{1}{n} \right\} \\
&= \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{p}_\tau(l) > \hat{p}_\tau(k) + \frac{1}{n} \right\}.
\end{aligned}$$

It follows that

$$\begin{aligned}
k \in \hat{C}_{\alpha;\tau} &\iff \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{p}_\tau(l) > \hat{p}_\tau(k) + \frac{1}{n} \right\} < (1-\alpha) \left(1 + \frac{1}{n} \right) \\
&\iff \hat{p}_\tau(k) \geq \hat{\ell}_{\alpha;\tau},
\end{aligned}$$

where the threshold $\hat{\ell}_{\alpha;\tau}$ is defined as

$$\hat{\ell}_{\alpha;\tau} := \inf \left\{ t \in [0, 1] : \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \{ \hat{p}_\tau(l) > t \} < (1-\alpha) \left(1 + \frac{1}{n} \right) \right\}. \quad (3)$$

How to compute $\hat{\ell}_{\alpha;\tau}$. The function $G : [0, 1] \rightarrow [0, 1]$, $t \mapsto \hat{G}_\tau(t) := \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \{ \hat{p}_\tau(l) > t \}$ is decreasing piece-wise constant right-continuous function which changes value at $\hat{p}_\tau(1), \dots, \hat{p}_\tau(K)$. Let $x_1 > \dots > x_\kappa$ be the distinct values among $\hat{p}_\tau(1), \dots, \hat{p}_\tau(K)$ sorted from largest to smallest, and for all $j \in \{1, \dots, \kappa\}$, $\rho_j := \sum_{k=1}^K \hat{p}_\tau(k) \mathbb{1} \{ \hat{p}_\tau(k) = x_j \}$. Consider the cumulative sum of $\rho_1, \dots, \rho_\kappa$, s_1, \dots, s_κ . It follows that $G(x_1) = 0$ and for every $j \in \{2, \dots, \kappa\}$

$$G(x_j) = \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \{ \hat{p}_\tau(l) > x_j \} = \sum_{l=1}^K \sum_{i=1}^{\kappa} \mathbb{1} \{ x_i = \hat{p}_\tau(l) \} \hat{p}_\tau(l) \mathbb{1} \{ \hat{p}_\tau(l) > x_j \}$$

$$= \sum_{i=1}^{\kappa} \rho_i \mathbb{1} \{x_i > x_j\} = \sum_{i=1}^{j-1} \rho_i = s_{j-1}.$$

It follows that, one only has to check for finite number of values

$$\begin{aligned} \hat{\ell}_{\alpha;\tau} &= \inf \left\{ t \in [0, 1] : \hat{G}_\tau(t) < (1 - \alpha) \left(1 + \frac{1}{n} \right) \right\} \\ &= \min \left\{ x_i : i \in \{1, \dots, \kappa\}, s_{i-1} < (1 - \alpha) \left(1 + \frac{1}{n} \right) \right\}. \end{aligned}$$

□

Proposition 2 (Instant-by-instant prediction upper band, MDist-full). *Let ξ_1, \dots, ξ_n be n independent copies of ξ . For any control level $\alpha \in [0, 1]$, the band $\hat{B}_\alpha^{\text{MDist-full,up}}$ defined as, for every $\tau \in \{1, \dots, T\}$*

$$\hat{B}_{\alpha;\tau}^{\text{MDist-full,up}} := \left\{ k \in \{1, \dots, K\} : k \leq \hat{Q}_\tau^{\text{up}} \left((1 - \alpha) \left(1 + \frac{1}{n} \right) \right) + 1 \right\} \quad (4)$$

ensures control of the instant-by-instant coverage of ξ at a control level α , the empirical marginal upper quantile function \hat{Q}_τ^{up} is defined in Equation (Eq. (6)).

Proof of Proposition 2. Let $\alpha \in [0, 1]$ and $\tau \in \{1, \dots, T\}$. A full conformal prediction region $\hat{C}_{\alpha;\tau}$ can be defined as

$$\hat{C}_{\alpha;\tau} := \{k \in \{1, \dots, K\} : \hat{\pi}(k) > \alpha\},$$

where for every $k \in \{1, \dots, K\}$

$$\hat{\pi}(k) := \frac{1 + \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_\tau^k(\xi_{i;\tau}) \geq \hat{F}_\tau^k(k) \right\}}{n + 1},$$

and for every $l \in \{1, \dots, K\}$

$$\hat{F}_\tau^k(l) := \frac{n}{n + 1} \hat{F}_\tau(l) + \frac{1}{n + 1} \mathbb{1} \{k \leq l\},$$

where the empirical marginal cumulative density function \hat{F}_τ is defined as

$$\hat{F}_\tau(l) := \frac{1}{n} \sum_{i=1}^n \mathbb{1} \{\xi_{i;\tau} \leq l\}. \quad (5)$$

Since $\xi_{1;\tau}, \dots, \xi_{n;\tau}$ are i.i.d. copies of ξ_τ , $\hat{C}_{\alpha;\tau}$ is a confidence prediction region (Vovk, Gamerman, and Shafer, 2005)

$$\mathbb{P} \left[\xi_\tau \in \hat{C}_{\alpha;\tau} \right] \geq 1 - \alpha.$$

Let us now provide an explicit expression of $\hat{C}_{\alpha;\tau}$.

$$\begin{aligned} k \in \hat{C}_{\alpha;\tau} &\iff \hat{\pi}_\tau(k) > \alpha \\ &\iff \frac{1 + \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_\tau^k(\xi_{i;\tau}) \geq \hat{F}_\tau^k(k) \right\}}{n + 1} > \alpha \end{aligned}$$

$$\iff \frac{1}{n} \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_\tau^k(\xi_{i;\tau}) < \hat{F}_\tau^k(k) \right\} < (1 - \alpha) \left(1 + \frac{1}{n} \right).$$

Let us focus on the l.h.s. term. Let us define the function $\hat{G}_\tau : \{1, \dots, K\} \rightarrow [0, 1]$ such that for every k

$$\begin{aligned} \hat{G}_\tau(k) &:= \frac{1}{n} \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_\tau^k(\xi_{i;\tau}) < \hat{F}_\tau^k(k) \right\} \\ &= \frac{1}{n} \sum_{i=1}^n \sum_{l=1}^K \mathbb{1} \{l = \xi_{i;\tau}\} \mathbb{1} \left\{ \hat{F}_\tau^k(\xi_{i;\tau}) < \hat{F}_\tau^k(k) \right\} \\ &= \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{F}_\tau^k(l) < \hat{F}_\tau^k(k) \right\} \\ &= \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \frac{n}{n+1} \hat{F}_\tau(l) + \frac{1}{n+1} \mathbb{1} \{k \leq l\} < \frac{n}{n+1} \hat{F}_\tau(k) + \frac{1}{n+1} \right\} \\ &= \sum_{l=1}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{F}_\tau(l) + \frac{1}{n} \mathbb{1} \{k \leq l\} < \hat{F}_\tau(k) + \frac{1}{n} \right\} \\ &= \sum_{l=1, l < k}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{F}_\tau(l) < \hat{F}_\tau(k) + \frac{1}{n} \right\} + \sum_{l=1, l \geq k}^K \hat{p}_\tau(l) \mathbb{1} \left\{ \hat{F}_\tau(l) < \hat{F}_\tau(k) \right\}. \end{aligned}$$

If $1 \leq l < k$ then $\hat{F}_\tau(l) \leq \hat{F}_\tau(k) < \hat{F}_\tau(k) + \frac{1}{n}$, and if $K \geq l \geq k$ then $\hat{F}_\tau(l) \geq \hat{F}_\tau(k)$. The above equation can be rewritten as

$$\hat{G}_\tau(k) = \sum_{l=1, l < k}^K \hat{p}_\tau(l) = \hat{F}_\tau(k-1).$$

Going back to trying to find an expression for $\hat{C}_{\alpha;\tau}$

$$\begin{aligned} k \in \hat{C}_{\alpha;\tau} &\iff \hat{F}_\tau(k-1) < (1 - \alpha) \left(1 + \frac{1}{n} \right) \\ &\iff k-1 \leq \hat{Q}_\tau \left((1 - \alpha) \left(1 + \frac{1}{n} \right) \right) \\ &\iff k \leq \hat{Q}_\tau \left((1 - \alpha) \left(1 + \frac{1}{n} \right) \right) + 1, \end{aligned}$$

where the empirical marginal upper quantile function is defined as, for every level $a \in [0, 1]$,

$$\hat{Q}_\tau^{\text{up}}(a) := \max \left\{ k \in \{1, \dots, K\} : \hat{F}_\tau(k) < a \right\} \quad (6)$$

the empirical marginal cumulative distribution function \hat{F}_τ in Equation (Eq. (5)). \square

Proposition 3 (Instant-by-instant prediction lower band, MDist-full). *Let ξ_1, \dots, ξ_n be n independent copies of ξ . For any control level $\alpha \in [0, 1]$, the band $\hat{B}_\alpha^{\text{MDist-full,lo}}$ defined as, for every $\tau \in \{1, \dots, T\}$*

$$\hat{B}_{\alpha;\tau}^{\text{MDist-full,lo}} := \left\{ k \in \{1, \dots, K\} : k \geq \hat{Q}_\tau^{\text{lo}} \left(\alpha \left(1 + \frac{1}{n} \right) - \frac{1}{n} \right) \right\} \quad (7)$$

ensures control of the instant-by-instant coverage of ξ at a control level α , where the marginal empirical lower quantile function \hat{Q}_τ^{lo} is defined in Equation (Eq. (8)).

Proof of Proposition 3. Let $\alpha \in [0, 1]$ and $\tau \in \{1, \dots, T\}$. A full conformal prediction region $\hat{C}_{\alpha;\tau}$ can be defined as

$$\hat{C}_{\alpha;\tau} := \{k \in \{1, \dots, K\} : \hat{\pi}(k) > \alpha\},$$

where

$$\hat{\pi}(k) := \frac{1 + \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_{\tau}^k(\xi_{i;\tau}) \leq \hat{F}_{\tau}^k(k) \right\}}{n+1}.$$

Since $\xi_{1;\tau}, \dots, \xi_{n;\tau}$ are i.i.d. copies of ξ_{τ} , $\hat{C}_{\alpha;\tau}$ is a confidence prediction region (Vovk, Gamerman, and Shafer, 2005)

$$\mathbb{P} \left[\xi_{\tau} \in \hat{C}_{\alpha;\tau} \right] \geq 1 - \alpha.$$

Let us now provide an explicit expression of $\hat{C}_{\alpha;\tau}$.

$$\begin{aligned} k \in \hat{C}_{\alpha;\tau} &\iff \hat{\pi}_{\tau}(k) > \alpha \\ &\iff \frac{1 + \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_{\tau}^k(\xi_{i;\tau}) \leq \hat{F}_{\tau}^k(k) \right\}}{n+1} > \alpha \\ &\iff \frac{1}{n} \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_{\tau}^k(\xi_{i;\tau}) \leq \hat{F}_{\tau}^k(k) \right\} > \alpha \left(1 + \frac{1}{n} \right) - \frac{1}{n}. \end{aligned}$$

Let us focus on the l.h.s. term. Let us define the function $\tilde{G}_{\tau} : \{1, \dots, K\} \rightarrow [0, 1]$ such that for every k

$$\begin{aligned} \tilde{G}_{\tau}(k) &:= \frac{1}{n} \sum_{i=1}^n \mathbb{1} \left\{ \hat{F}_{\tau}^k(\xi_{i;\tau}) \leq \hat{F}_{\tau}^k(k) \right\} \\ &= \frac{1}{n} \sum_{i=1}^n \sum_{l=1}^K \mathbb{1} \{l = \xi_{i;\tau}\} \mathbb{1} \left\{ \hat{F}_{\tau}^k(\xi_{i;\tau}) \leq \hat{F}_{\tau}^k(k) \right\} \\ &= \sum_{l=1}^K \hat{p}_{\tau}(l) \mathbb{1} \left\{ \hat{F}_{\tau}^k(l) \leq \hat{F}_{\tau}^k(k) \right\} \\ &= \sum_{l=1}^K \hat{p}_{\tau}(l) \mathbb{1} \left\{ \frac{n}{n+1} \hat{F}_{\tau}(l) + \frac{1}{n+1} \mathbb{1} \{k \leq l\} \leq \frac{n}{n+1} \hat{F}_{\tau}(k) + \frac{1}{n+1} \right\} \\ &= \sum_{l=1}^K \hat{p}_{\tau}(l) \mathbb{1} \left\{ \hat{F}_{\tau}(l) + \frac{1}{n} \mathbb{1} \{k \leq l\} \leq \hat{F}_{\tau}(k) + \frac{1}{n} \right\} \\ &= \sum_{l=1, l \leq k}^K \hat{p}_{\tau}(l) \mathbb{1} \left\{ \hat{F}_{\tau}(l) \leq \hat{F}_{\tau}(k) + \frac{1}{n} \right\} + \sum_{l=1, l > k}^K \hat{p}_{\tau}(l) \mathbb{1} \left\{ \hat{F}_{\tau}(l) \leq \hat{F}_{\tau}(k) \right\}. \end{aligned}$$

If $1 \leq l < k$ then $\hat{F}_{\tau}(l) \leq \hat{F}_{\tau}(k) < \hat{F}_{\tau}(k) + \frac{1}{n}$, and if $K \geq l > k$ and $\hat{p}_{\tau}(l) \neq 0$, then

$$\hat{F}_{\tau}(l) = \sum_{\tilde{l}=1}^l \hat{p}_{\tau}(\tilde{l}) = \sum_{\tilde{l}=1}^k \hat{p}_{\tau}(\tilde{l}) + \sum_{\tilde{l}=k+1}^l \hat{p}_{\tau}(\tilde{l}) = \hat{F}_{\tau}(k) + \sum_{\tilde{l}=k+1}^l \hat{p}_{\tau}(\tilde{l}) > \hat{F}_{\tau}(k),$$

since $\sum_{l=k+1}^l \hat{p}_\tau(\hat{l})$ includes $\hat{p}_\tau(l) \neq 0$. Hence, the function \tilde{G}_τ can be rewritten as

$$\tilde{G}_\tau(k) = \sum_{l=1, l \leq k}^K \hat{p}_\tau(l) = \hat{F}_\tau(k).$$

Going back to trying to find an expression for $\hat{C}_{\alpha;\tau}$

$$\begin{aligned} k \in \hat{C}_{\alpha;\tau} &\iff \hat{F}_\tau(k) > \alpha \left(1 + \frac{1}{n}\right) - \frac{1}{n} \\ &\iff k \geq \tilde{Q}_\tau \left(\alpha \left(1 + \frac{1}{n}\right) - \frac{1}{n} \right), \end{aligned}$$

where the empirical marginal lower quantile function is defined as, for every level $a \in (0, 1)$

$$\tilde{Q}_\tau^{\text{lo}}(a) := \min \left\{ k \in \{1, \dots, K\} : \hat{F}_\tau(k) > a \right\}, \quad (8)$$

the empirical marginal cumulative distribution function \hat{F}_τ in Equation (Eq. (5)). \square

Proposition 4 (Instant-by-instant prediction band, MDist-full). *Let ξ_1, \dots, ξ_n be n independent copies of ξ . For any control level $\alpha \in [0, 1]$, and for any $\alpha_{\text{lo}}, \alpha_{\text{up}} \in [0, 1]$ such that $\alpha_{\text{lo}} + \alpha_{\text{up}} = \alpha$, the band $\hat{B}_\alpha^{\text{MDist-full}}$ defined as, for every $\tau \in \{1, \dots, T\}$*

$$\begin{aligned} \hat{B}_{\alpha;\tau}^{\text{MDist-full}} := \left\{ k \in \{1, \dots, K\} : \hat{Q}_\tau^{\text{lo}} \left(\alpha_{\text{lo}} \left(1 + \frac{1}{n}\right) - \frac{1}{n} \right) \leq k, \right. \\ \left. k \leq \hat{Q}_\tau^{\text{up}} \left((1 - \alpha_{\text{up}}) \left(1 + \frac{1}{n}\right) \right) + 1 \right\}, \end{aligned} \quad (9)$$

ensures control of the instant-by-instant coverage of ξ at a control level α .

Proof of Proposition 4. Let $\alpha \in [0, 1]$ and $\tau \in \{1, \dots, T\}$. It follows from union bound that

$$\begin{aligned} \mathbb{P} \left[\xi_\tau \in \hat{B}_{\alpha;\tau}^{\text{MDist-full}} \right] &= \mathbb{P} \left[\xi_\tau \in \hat{B}_{\alpha_{\text{up}};\tau}^{\text{MDist-full,up}} \cap \hat{B}_{\alpha_{\text{lo}};\tau}^{\text{MDist-full,lo}} \right] \\ &= 1 - \mathbb{P} \left[\xi_\tau \in \left(\hat{B}_{\alpha_{\text{up}};\tau}^{\text{MDist-full,up}} \right)^c \cup \left(\hat{B}_{\alpha_{\text{lo}};\tau}^{\text{MDist-full,lo}} \right)^c \right] \\ &\geq 1 - \left(\mathbb{P} \left[\xi_\tau \in \left(\hat{B}_{\alpha_{\text{up}};\tau}^{\text{MDist-full,up}} \right)^c \right] + \mathbb{P} \left[\xi_\tau \in \left(\hat{B}_{\alpha_{\text{lo}};\tau}^{\text{MDist-full,lo}} \right)^c \right] \right) \\ &\geq 1 - (\alpha_{\text{up}} + \alpha_{\text{lo}}) = 1 - \alpha. \end{aligned}$$

\square

Proposition 5 (Instant-by-instant prediction band, MDist-Split). *Let ξ_1, \dots, ξ_n be n independent copies of ξ . Let I_1 and I_2 be two index sets with cardinal n_1 and n_2 respectively such that $I_1 \sqcup I_2 = \{1, \dots, n\}$. For any control level $\alpha \in [0, 1]$, the band $\hat{B}_\alpha^{\text{MDist-split}}$ defined as, for every $\tau \in \{1, \dots, T\}$*

$$\hat{B}_{\alpha;\tau}^{\text{MDist-split}} := \left\{ k \in \{1, \dots, K\} : \tilde{Q}_{D_1;\tau}^{\text{lo}} \left(\hat{t}_{\alpha;\tau}^{\text{MDist-split}} \right) \leq k \leq \tilde{Q}_{D_1;\tau}^{\text{up}} \left(1 - \hat{t}_{\alpha;\tau}^{\text{MDist-split}} \right) \right\}, \quad (10)$$

ensures control of the instant-by-instant coverage of ξ at a control level α , where the threshold $\hat{t}_{\alpha;\tau}^{\text{MDist-split}}$ is defined in Equation (Eq. (12)) and the marginal empirical upper and lower quantile function $\tilde{Q}_{D_1;\tau}^{\text{up}}$ and $\tilde{Q}_{D_1;\tau}^{\text{lo}}$ are defined in Equations (Eq. (13)) and (Eq. (14)) respectively.

Proof of Proposition 5. Let $\tau \in \{1, \dots, T\}$. Define the empirical marginal cumulative density function $\hat{F}_{D_1;\tau}$ trained on the data set $D_1 := \{\xi_i, i \in I_1\}$ as, for every $k \in \{1, \dots, K\}$

$$\hat{F}_{D_1;\tau}(k) := \frac{1}{n_1} \sum_{i \in I_1} \mathbb{1}\{\xi_{i;\tau} \leq k\}. \quad (11)$$

Upon the dataset $D_2 := \{\xi_i, i \in I_2\}$, one can define split conformal prediction region $\hat{C}_{\alpha;\tau}$ as

$$\hat{C}_{\alpha;\tau} := \{k \in \{1, \dots, K\} : \hat{\pi}_{D_2,\tau}(k) > \alpha\},$$

where for every $k \in (1, \dots, K)$

$$\hat{\pi}_{D_2,\tau}(k) := \frac{1 + \sum_{i \in I_2} \mathbb{1}\{\hat{A}_{D_1;\tau}(\xi_{i;\tau}) \leq \hat{A}_{D_1;\tau}(k)\}}{1 + n_2},$$

where the conformity score $\hat{A}_{D_1;\tau}(k) := \min(\hat{F}_{D_1;\tau}(k), 1 - \hat{F}_{D_1;\tau}(k))$. Since $\xi_{1;\tau}, \dots, \xi_{n_2;\tau}$ are i.i.d. copies of ξ_τ , it follows that $\hat{C}_{\alpha;\tau}$ is a confidence prediction region

$$\mathbb{P}(\xi_\tau \in \hat{C}_{\alpha;\tau}) \geq 1 - \alpha.$$

Let us now compute an explicit expression for $\hat{C}_{\alpha;\tau}$.

$$\begin{aligned} k &\in \hat{C}_{\alpha;\tau} \\ \iff \frac{1 + \sum_{i \in I_2} \mathbb{1}\{\hat{A}_{D_1;\tau}(\xi_{i;\tau}) \leq \hat{A}_{D_1;\tau}(k)\}}{1 + n_2} &> \alpha \\ \iff \frac{1}{n_2} \sum_{i \in I_2} \mathbb{1}\{\hat{A}_{D_1;\tau}(\xi_{i;\tau}) \leq \hat{A}_{D_1;\tau}(k)\} &> \alpha \left(1 + \frac{1}{n_2}\right) - \frac{1}{n_2} \\ \iff \hat{A}_{D_1;\tau}(k) &\geq \hat{\ell}_{\alpha;\tau}, \end{aligned}$$

where the level $\hat{t}_{\alpha;\tau}^{\text{MDist-split}}$ is defined as

$$\begin{aligned} \hat{t}_{\alpha;\tau}^{\text{MDist-split}} &:= \inf \left\{ t \in [0, 1] : \frac{1}{n_2} \sum_{i \in I_2} \mathbb{1}\{\hat{A}_{D_1;\tau}(\xi_{i;\tau}) \leq t\} > \alpha \left(1 + \frac{1}{n_2}\right) - \frac{1}{n_2} \right\} \\ &= \hat{A}_{D_1;\tau}(\xi_{(i_{n_2;\alpha}),\tau}), \end{aligned} \quad (12)$$

where the index $i_{n_2;\alpha} := \lceil \alpha(n_2 + 1) - 1 \rceil$, and $\hat{A}_{D_1;\tau}(\xi_{(1);\tau}) \leq \dots \leq \hat{A}_{D_1;\tau}(\xi_{(n_2);\tau})$ are the conformity scores sorted in increasing order. Going back to trying to find an expression of the prediction region

$$\begin{aligned} k &\in \hat{C}_{\alpha;\tau} \\ \iff \min(\hat{F}_{D_1;\tau}(k), 1 - \hat{F}_{D_1;\tau}(k)) &\geq \hat{t}_{\alpha;\tau}^{\text{MDist-split}}, \\ \iff \hat{F}_{D_1;\tau}(k) \geq \hat{t}_{\alpha;\tau}^{\text{MDist-split}}, \text{ and } 1 - \hat{F}_{D_1;\tau}(k) &\geq \hat{t}_{\alpha;\tau}^{\text{MDist-split}}, \\ \iff \hat{t}_{\alpha;\tau}^{\text{MDist-split}} \leq \hat{F}_{D_1;\tau}(k) \leq 1 - \hat{t}_{\alpha;\tau}^{\text{MDist-split}}, \\ \iff \tilde{Q}_{D_1;\tau}^{\text{lo}}(\hat{t}_{\alpha;\tau}^{\text{MDist-split}}) \leq k \leq \tilde{Q}_{D_1;\tau}^{\text{up}}(1 - \hat{t}_{\alpha;\tau}^{\text{MDist-split}}), \end{aligned}$$

where the empirical marginal upper quantile function built from D_1 is defined as, for every level $a \in [0, 1]$ is defined as

$$\tilde{Q}_{D_1;\tau}^{\text{up}}(1-a) := \max \left\{ k \in \{1, \dots, K\} : \hat{F}_{D_1;\tau}(k) \leq 1-a \right\}, \quad (13)$$

as for the lower one

$$\tilde{Q}_{D_1;\tau}^{\text{lo}}(a) := \min \left\{ k \in \{1, \dots, K\} : \hat{F}_{D_1;\tau}(k) \geq a \right\}. \quad (14)$$

□

Proposition 6 (γ -simultaneous band). *Let ξ_1, \dots, ξ_n be i.i.d. copies of ξ . Let I_1 and I_2 be two index sets with cardinal n_1 and n_2 respectively such that $I_1 \sqcup I_2 = \{1, \dots, n\}$. Let $\hat{A}_{D_1;\tau} : \{1, \dots, K\} \rightarrow \mathbb{R}$, $k \mapsto \hat{A}_{D_1;\tau}(k)$ be a conformity-measure over $\{1, \dots, K\}$ built from the dataset $D_1 := \{\xi_i : i \in I_1\}$.*

For any slack level $\gamma \in [0, 1]$, control level $\alpha \in [0, 1]$, the prediction band $\hat{B}_{\gamma;\alpha}$ defined as for every $\tau \in \{1, \dots, T\}$

$$\hat{B}_{\gamma;\alpha;\tau} := \left\{ k \in \{1, \dots, K\} : \hat{A}_{D_1;\tau}(k) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right\}$$

ensures control of the γ -simultaneous coverage of ξ at a level α where the cut-off level $\hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})})$ is defined in Equation (Eq. 16) from the conformity score defined in Equation (Eq. 15).

Proof of Proposition 6. Let $\gamma \in [0, 1]$ and $\alpha \in [0, 1]$. One can define a conformity measure $\hat{t}_{D_1;\gamma} : \{1, \dots, K\}^T \rightarrow \mathbb{R}$ such that for every $\xi \in \{1, \dots, K\}^T$

$$\hat{t}_{D_1;\gamma}(\xi) := \sup \left\{ t \in \mathbb{R} : \frac{1}{T} \sum_{\tau=1}^T \mathbb{1} \left\{ \hat{A}_{D_1;\tau}(\xi_\tau) \geq t \right\} \geq 1-\gamma \right\} = \hat{A}_{D_1;(\tau_{\gamma,T})}(\xi_{(\tau_{\gamma,T})}), \quad (15)$$

where $\hat{A}_{D_1;(1)}(\xi_{(1)}) \geq \dots \geq \hat{A}_{D_1;(T)}(\xi_{(T)})$ are sorted in decreasing order and $\tau_{\gamma,T} := \lceil T(1-\gamma) \rceil$. Upon the dataset $D_2 := \{\xi_i : i \in I_2\}$, one can define a split conformal prediction region as

$$\hat{C}_{\gamma;\alpha} := \left\{ \xi \in \{1, \dots, K\}^T : \hat{\pi}_{D_2}(\xi) > \alpha \right\},$$

where for every $\xi \in \{1, \dots, K\}^T$

$$\hat{\pi}_{D_2}(\xi) := \frac{1 + \sum_{i \in I_2} \{\hat{t}_{D_1;\gamma}(\xi_i) \leq \hat{t}_{D_1;\gamma}(\xi)\}}{n_2 + 1}.$$

Let us now provide an explicit expression for $\hat{C}_{\gamma;\alpha}$,

$$\begin{aligned} \xi \in \hat{C}_{\gamma;\alpha} &\iff \frac{1 + \sum_{i \in I_2} \{\hat{t}_{D_1;\gamma}(\xi_i) \leq \hat{t}_{D_1;\gamma}(\xi)\}}{n_2 + 1} > \alpha \\ &\iff \frac{1}{n_2} \sum_{i \in I_2} \{\hat{t}_{D_1;\gamma}(\xi_i) \leq \hat{t}_{D_1;\gamma}(\xi)\} > \left(1 + \frac{1}{n_2}\right) \alpha - \frac{1}{n_2} \\ &\iff \hat{t}_{D_1;\gamma}(\xi) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}), \end{aligned} \quad (16)$$

where $\hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \leq \dots \leq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})})$ are sorted in increasing order and $i_{n_2;\alpha} := \lceil (n_2 + 1) \alpha - 1 \rceil$. Hence, the prediction band $\hat{B}_{\gamma;\alpha}$ defined as for every $\tau \in \{1, \dots, T\}$

$$\hat{B}_{\gamma;\alpha;\tau} := \left\{ k \in \{1, \dots, K\} : \hat{A}_{D_1;\tau}(k) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right\}$$

ensures the following

$$\begin{aligned}
\mathbb{P} \left[\frac{1}{T} \sum_{\tau=1}^T \mathbb{1} \left\{ \xi_{\tau} \in \hat{B}_{\gamma;\alpha;\tau} \right\} \right] &= \mathbb{P} \left[\frac{1}{T} \sum_{\tau=1}^T \mathbb{1} \left\{ \hat{A}_{D_1;\tau}(\xi_{\tau}) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right\} \right] \\
&= \mathbb{P} \left[\hat{t}_{D_1;\gamma}(\xi) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right] \\
&= \mathbb{P} \left[\xi \in \hat{C}_{\gamma,\alpha} \right] \geq 1 - \alpha.
\end{aligned}$$

□

Corollary 1 (γ -simultaneous band, MD-Split). *Let ξ_1, \dots, ξ_n be i.i.d. copies of ξ . Let I_1 and I_2 be two index sets with cardinal n_1 and n_2 respectively such that $I_1 \sqcup I_2 = \{1, \dots, n\}$.*

For any slack $\gamma \in (0, 1)$, control level $\alpha \in [0, 1]$, the prediction band $\hat{B}_{\gamma;\alpha}^{\text{MD-split}}$ such that for every $\tau \in \{1, \dots, T\}$

$$\hat{B}_{\gamma;\alpha;\tau}^{\text{MD-split}} := \left\{ k \in \{1, \dots, K\} : \hat{p}_{D_1;\tau}(k) \geq \hat{\ell}_{\gamma;\alpha}^{\text{MD-Split}} \right\}, \quad (17)$$

ensures control of γ -simultaneous coverage of ξ at a control level α , where empirical marginal probability density function $\hat{p}_{D_1;\tau}$ is defined in Equation (Eq. (18)), and the threshold is $\hat{\ell}_{\gamma;\alpha}^{\text{MD-Split}}$ is defined in Equation (Eq. (19)).

Proof of Corollary 1. For every $\tau \in \{1, \dots, K\}$, define empirical marginal probability density function $\hat{p}_{D_1;\tau}$ built from the dataset $D_1 := \{\xi_i : i \in I_1\}$ as, for every $k \in \{1, \dots, K\}$

$$\hat{p}_{D_1;\tau}(k) := \frac{1}{n_1} \sum_{i \in I_1} \mathbb{1} \{ \xi_{i;\tau} = k \}. \quad (18)$$

Applying Proposition 6 by choosing for every $\tau \in \{1, \dots, T\}$, and every $k \in \{1, \dots, K\}$, $\hat{A}_{D_1;\tau}(k) := \hat{p}_{D_1;\tau}(k)$, the prediction band $\hat{B}_{\gamma;\alpha}^{\text{MD-split}}$ defined as, for every $\tau \in \{1, \dots, T\}$

$$\begin{aligned}
\hat{B}_{\gamma;\alpha;\tau}^{\text{MD-split}} &:= \left\{ k \in \{1, \dots, K\} : \hat{A}_{D_1;\tau}(k) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right\} \\
&= \left\{ k \in \{1, \dots, K\} : \hat{p}_{D_1;\tau}(k) \geq \hat{\ell}_{\gamma;\alpha}^{\text{MD-Split}} \right\},
\end{aligned}$$

ensures control of γ -simultaneous coverage of ξ at a control level α , where the threshold $\hat{\ell}_{\gamma;\alpha}^{\text{MD-Split}}$ is defined as

$$\hat{\ell}_{\gamma;\alpha}^{\text{MD-Split}} := \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}). \quad (19)$$

□

Corollary 2 (γ -simultaneous band, MHPD-Split). *Let ξ_1, \dots, ξ_n be i.i.d. copies of ξ . Let I_1 and I_2 be two index sets with cardinal n_1 and n_2 respectively such that $I_1 \sqcup I_2 = \{1, \dots, n\}$.*

For any slack $\gamma \in (0, 1)$, control level $\alpha \in [0, 1]$, the prediction band $\hat{B}_{\gamma;\alpha}^{\text{MHPD-split}}$ such that for every $\tau \in \{1, \dots, T\}$

$$\hat{B}_{\gamma;\alpha;\tau}^{\text{MHPD-split}} := \left\{ k \in \{1, \dots, K\} : \hat{p}_{D_1;\tau}(k) > \hat{\ell}_{\gamma;\alpha;\tau}^{\text{MHPD-split}} \right\}, \quad (20)$$

ensures γ -simultaneous coverage of ξ at a control level α , where empirical marginal probability density function $\hat{p}_{D_1;\tau}$ is defined in Equation (Eq. (18)), and the threshold $\hat{\ell}_{\gamma;\alpha;\tau}^{\text{MHPD-split}}$ is defined in Equation (Eq. (22)).

Proof of Corollary 2. For every $\tau \in \{1, \dots, K\}$, and every $k \in \{1, \dots, K\}$ define the rank $\hat{R}_{D_1;\tau}(k)$ of k at the instant τ built from the dataset $D_1 := \{\xi_i : i \in I_1\}$ as

$$\hat{R}_{D_1;\tau}(k) := \sum_{l=1}^K \hat{p}_{D_1;\tau}(l) \mathbb{1} \{ \hat{p}_{D_1;\tau}(l) \leq \hat{p}_{D_1;\tau}(k) \}. \quad (21)$$

Applying Proposition 6 by choosing for every $\tau \in \{1, \dots, T\}$, and every $k \in \{1, \dots, K\}$, $\hat{A}_{D_1;\tau}(k) := \hat{R}_{D_1;\tau}(k)$, the prediction band $\hat{B}_{\gamma;\alpha}^{\text{MD-split}}$ defined as, for every $\tau \in \{1, \dots, T\}$

$$\begin{aligned} \hat{B}_{\gamma;\alpha;\tau}^{\text{MHPD-split}} &:= \left\{ k \in \{1, \dots, K\} : \hat{A}_{D_1;\tau}(k) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right\} \\ &= \left\{ k \in \{1, \dots, K\} : \hat{R}_{D_1;\tau}(k) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right\} \\ &= \left\{ k \in \{1, \dots, K\} : \hat{p}_{D_1;\tau}(k) > \hat{\ell}_{\gamma;\alpha;\tau}^{\text{MHPD-split}} \right\}, \end{aligned}$$

ensures control of γ -simultaneous coverage of ξ at a control level α , where the cut-off $\hat{\ell}_{\gamma;\alpha;\tau}^{\text{MHPD-split}}$ is defined as

$$\hat{\ell}_{\gamma;\alpha;\tau}^{\text{MHPD-split}} := \sup \left\{ \ell \in [0, 1] : \sum_{l=1}^K \hat{p}_{D_1;\tau}(l) \mathbb{1} \{ \hat{p}_{D_1;\tau}(l) > \ell \} > 1 - \hat{t}_{D_1;\gamma}^{\text{MHPD-split}}(\xi_{(i_{n_2;\alpha})}) \right\}, \quad (22)$$

□

Corollary 3 (γ -simultaneous band, MDist-Split). *Let ξ_1, \dots, ξ_n be n independent copies of ξ . Let I_1 and I_2 be two index sets with cardinal n_1 and n_2 respectively such that $I_1 \sqcup I_2 = \{1, \dots, n\}$.*

For any slack $\gamma \in (0, 1)$, any control level $\alpha \in [0, 1]$, the band $\hat{B}_{\gamma;\alpha}^{\text{MDist-split}}$ defined as, for every $\tau \in \{1, \dots, T\}$

$$\hat{B}_{\gamma;\alpha;\tau}^{\text{MDist-split}} := \left\{ k \in \{1, \dots, K\} : \hat{Q}_{D_1,\tau}^{\text{lo}}(\hat{t}_{\gamma;\alpha}^{\text{MDist-split}}) \leq k \leq \hat{Q}_{D_1,\tau}^{\text{lo}}(1 - \hat{t}_{\gamma;\alpha}^{\text{MDist-split}}) \right\}, \quad (23)$$

ensures γ -simultaneous coverage of ξ at a control level α , where the level $\hat{t}_{\gamma;\alpha}^{\text{MDist-split}}$ is defined in Equation (Eq. (25)).

Proof of Corollary 3. Applying Proposition 6, for every $\tau \in \{1, \dots, K\}$, and $k \in \{1, \dots, K\}$

$$\hat{A}_{D_1;\tau}(k) := \min \left(\hat{F}_{D_1;\tau}(k), 1 - \hat{F}_{D_1;\tau}(k) \right), \quad (24)$$

the prediction band $\hat{B}_{\gamma;\alpha}^{\text{MDist-split}}$ defined as, for every $\tau \in \{1, \dots, T\}$

$$\begin{aligned} \hat{B}_{\gamma;\alpha;\tau}^{\text{MHPD-split}} &:= \left\{ k \in \{1, \dots, K\} : \hat{A}_{D_1;\tau}(k) \geq \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}) \right\} \\ &= \left\{ k \in \{1, \dots, K\} : \min \left(\hat{F}_{D_1;\tau}(k), 1 - \hat{F}_{D_1;\tau}(k) \right) \geq \hat{t}_{\gamma;\alpha}^{\text{MDist-split}} \right\} \\ &= \left\{ k \in \{1, \dots, K\} : \hat{Q}_{D_1,\tau}^{\text{lo}}(\hat{t}_{\gamma;\alpha}^{\text{MDist-split}}) \leq k \leq \hat{Q}_{D_1,\tau}^{\text{lo}}(1 - \hat{t}_{\gamma;\alpha}^{\text{MDist-split}}) \right\}, \end{aligned}$$

ensures control of γ -simultaneous coverage of ξ at a control level α , where the level $\hat{t}_{\gamma;\alpha}^{\text{MDist-split}}$ is defined as

$$\hat{t}_{\gamma;\alpha}^{\text{MDist-split}} := \hat{t}_{D_1;\gamma}(\xi_{(i_{n_2;\alpha})}). \quad (25)$$

□

Proposition 7 (Make it high probability.). *Let ξ_1, \dots, ξ_n be n independent copies of ξ . Let I_1 and I_2 be two index sets with cardinal n_1 and n_2 respectively such that $I_1 \sqcup I_2 = \{1, \dots, n\}$. For any risk level δ and a control level δ ,*

$$\mathbb{P} \left[\mathbb{P} \left[\xi \in \hat{C}_{a_{n_2; \alpha; \delta}} \mid D_2 \right] \geq 1 - \alpha \right] \geq 1 - \delta,$$

where the level $a_{n_2; \alpha; \delta}$ is given by

$$a_{n_2; \alpha; \delta}$$

Proof.

$$\mathbb{P} \left[\mathbb{P} [\mid D_2] \geq 1 - \alpha \right] \geq 1 - \delta.$$

□