Proofs for the paper "Flexible distribution-free conditional predictive bands using density estimators"

Definition 5.1. Whenever $\widehat{F}$ is a cdf, $\widehat{F}^{-1}$ refers to the generalized inverse of $\widehat{F}$.

Definition 5.2. $U_{\lfloor \alpha \rfloor}$ and $U_{\lceil \alpha \rceil}$ are the $\lfloor n^{-1}(n\alpha) \rfloor$ $\lceil n^{-1}(n\alpha) \rceil$ empirical quantiles of $U_1, \ldots, U_n$,

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Proof of Theorem 2.2. Let $U_i = \widehat{F}(Y_i|\mathbf{X}_i)$. Since $(\mathbf{X}_i, Y_i)$ are i.i.d. continuous random variables and $\widehat{F}$ is continuous, obtain that U_i are i.i.d. continuous random variables.

$$1 - \alpha \le \mathbb{P}\left(U_{n+1} \in [U_{\lfloor 0.5\alpha \rfloor}; U_{\lceil 1-0.5\alpha \rceil}]\right) \le 1 - \alpha + (n+1)^{-1}.$$

The conclusion follows from noticing that

$$\begin{aligned}&\mathbb{P}\left(U_{n+1} \in [U_{\lfloor 0.5\alpha \rfloor}; U_{\lceil 1-0.5\alpha \rceil}]\right)\\ =&\mathbb{P}\left(Y_{n+1} \in [\widehat{F}^{-1}(U_{\lfloor 0.5\alpha \rfloor}|\mathbf{X}_{n+1}); \widehat{F}^{-1}(U_{\lceil 1-0.5\alpha \rceil}|\mathbf{X}_{n+1})]\right)\\ =&\mathbb{P}(Y_{n+1} \in C(\mathbf{X}_{n+1}))\end{aligned}$$

□

Lemma 5.3. *Let $I_1 = \left\{i \le n : |\widehat{F}(Y_i|\mathbf{X}_i) - F(Y_i|\mathbf{X}_i)| < \eta_n^{1/3}\right\}$ and $I_2 = \{1, \ldots, n\} - I_1$. Under Assumption 2.3, $|I_2| = o_P(n)$ and $|I_1| = n + o_P(n)$.*

Proof. Let $A_n = \left\{\mathbb{E}\left[\sup_{y \in \mathcal{Y}} \left(\widehat{F}(y|\mathbf{X}) - F(y|\mathbf{X})\right)^2 \big| \widehat{F}\right] \ge \eta_n\right\}$ and $B_n = \left\{|\widehat{F}(Y|\mathbf{X}) - F(Y|\mathbf{X})| \ge \eta_n^{1/3}\right\}$.

$$\begin{aligned}\mathbb{P}(B_n) &= \mathbb{E}[\mathbb{P}(B_n|\widehat{F})\mathbb{I}(A_n)] + \mathbb{E}[\mathbb{P}(B_n|\widehat{F})\mathbb{I}(A_n^c)]\\ &\le \mathbb{P}(A_n) + \mathbb{E}\left[\frac{\mathbb{E}[(\widehat{F}(Y|\mathbf{X}) - F(Y|\mathbf{X}))^2|\widehat{F}]}{\eta_n^{2/3}}\mathbb{I}(A_n^c)\right]\\ &\le \rho_n + \eta_n^{1/3} = o(1)\end{aligned}$$

Note that $|I_2| \sim \text{Binomial}(n, \mathbb{P}(B_n))$. Since $\mathbb{P}(B_n) = o(1)$, conclude that $|I_2| = o_P(n)$. That is, $|I_1| = n + o_P(n)$. □

Lemma 5.4. *Under Assumption 2.3, If $U_i = \widehat{F}(Y_i|\mathbf{X}_i)$, then for every $\alpha \in (0,1)$, $U_{\lfloor \alpha \rfloor} = \alpha + o_P(1) = U_{\lceil \alpha \rceil}$.*

Proof. Let I_1 and I_2 be such as in Lemma 5.3. Also, let $\hat{G}_1$, G_1 and G_0 be, the empirical quantiles of, respectively, $\{U_i : i \in I_1\}$, $\{F(Y_i|\mathbf{X}_i) : i \in I_1\}$, and $\{F(Y_i|\mathbf{X}_i) : i \le n\}$. By definition of I_1, for every $\alpha^* \in [0,1]$, $\hat{G}_1^{-1}(\alpha^*) = G_1^{-1}(\alpha^*) + o(1)$. Also, $G_0^{-1}(\alpha^*) = \alpha^* + o_P(1)$. Therefore, since

$$G_0^{-1}\left(\frac{|I_1|\alpha^*}{n}\right) \le G_1^{-1}(\alpha^*) \le G_0^{-1}\left(\frac{|I_1|\alpha^* + |I_2|}{n}\right),$$

conclude that $\hat{G}_1^{-1}(\alpha^*) = \alpha^* + o_P(1)$. Finally, since

$$\hat{G}^{-1}\left(\frac{n\alpha - |I_2|}{|I_1|}\right) \le U_{\lfloor \alpha \rfloor} \le U_{\lceil \alpha \rceil} \le \hat{G}^{-1}\left(\frac{n\alpha}{|I_1|}\right),$$

Conclude that $U_{\lfloor \alpha \rfloor} = \alpha + o_P(1) = U_{\lceil \alpha \rceil}$. □

Lemma 5.5. *Let $U_i = \hat{F}(Y_i|\mathbf{X}_i)$. Under Assumptions 2.3 and 2.4,*

$$\begin{aligned}\widehat{F}^{-1}(U_{[0.5\alpha]}|\mathbf{X}_{n+1}) &= F^{-1}(0.5\alpha|\mathbf{X}_{n+1}) + o_P(1)\\ \widehat{F}^{-1}(U_{[1-0.5\alpha]}|\mathbf{X}_{n+1}) &= F^{-1}(1-0.5\alpha|\mathbf{X}_{n+1}) + o_P(1)\end{aligned}$$

Proof. In order to prove the first equality, it is enough to show that $F^{-1}(U_{[0.5\alpha]}|\mathbf{X}_{n+1}) = F^{-1}(0.5\alpha|\mathbf{X}_{n+1}) + o_P(1)$ and that $\widehat{F}^{-1}(U_{[0.5\alpha]}|\mathbf{X}_{n+1}) = F^{-1}(U_{[0.5\alpha]}|\mathbf{X}_{n+1}) + o_P(1)$. The first part follows from Lemma 5.4 and the continuity of $F(y|\mathbf{x})$ (Assumption 2.4). For the second part, note that, if $\sup_y |\hat{F}(y|\mathbf{x}) - F(y|\mathbf{x})| < \eta_n$, then, for every α^*, $|\hat{F}^{-1}(\alpha^*) - F^{-1}(\alpha^*)| \le \eta_n \left(\inf_y \frac{dF(y|\mathbf{x})}{dy}\right)^{-1}$. Using this observation, the proof of the second part follows from Assumption 2.4, and observing that $U_{[0.5\alpha]} = 0.5\alpha + o_P(1)$ (Lemma 5.4) and $\mathbb{P}(\sup_y |\hat{F}(y|\mathbf{x}) - F(y|\mathbf{x})| \ge \eta_n) = o(1)$ (Assumption 2.3).

The proof for the $1 - .5\alpha$ quantile is analogous to the one for the $.5\alpha$ quantile. □

Proof of Theorem 2.5. Follows directly from Lemma 5.5. □

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Proof Theorem 3.3. Let $\{i_1, \ldots, i_{n_j}\} = \{i : \mathbf{X}_i \in A(\mathbf{x}_{n+1})\}$, $U_l = \widehat{f}(Y_{i_l}|\mathbf{X}_{i_l})$, for $l = 1, \ldots, n_j$, and $U_{n_j+1} = \widehat{f}(Y_{n+1}|\mathbf{X}_{n+1})$. Since $(\mathbf{X}_1, Y_1), \ldots, (\mathbf{X}_{n_j}, Y_{n_j}), (\mathbf{X}_{n+1}, Y_{n+1})$ are i.i.d. random variables, obtain that U_i are i.i.d. random variables conditional on the event $\mathbf{X}_{n+1} \in A(\mathbf{x}_{n+1})$ and on $i_1, \ldots, i_{n_j}$. Therefore,

$$1 - \alpha \le \mathbb{P}\left(U_{m+1} \ge U_{\lfloor \alpha \rfloor} | \mathbf{X}_{n+1} \in A(\mathbf{x}_{n+1}), i_1, \ldots, i_{n_j}\right)$$

The conclusion follows from the fact that $Y_{n+1} \in C(\mathbf{X}_{n+1}) \iff U_{m+1} \ge U_{\lfloor 1-\alpha \rfloor}$ and because this holds for every sequence $i_1, \ldots, i_{n_j}$. □

Proof of Theorem 3.8. Let $U_i := f(Y_i|\mathbf{x}_i)$, $i = 1, \ldots, m$, $U_{n+1} := f(Y_{n+1}|\mathbf{x}_{n+1})$, and $W := (\mathbf{x}_1, \ldots, \mathbf{x}_m, \mathbf{x}_{n+1})$. If $g_{\mathbf{x}_i} = g_{\mathbf{x}_{n+1}}$ for every $i = 1, \ldots, m$, then $U_1, \ldots, U_m, U_{n+1}$ are i.i.d. conditional on W. Indeed, for every $t \in \mathbb{R}$,

$$\begin{aligned}\mathbb{P}(U_i \ge t|W) &= \mathbb{P}(f(Y_i|\mathbf{x}_i) \ge t|\mathbf{x}_i)\\ &= \mathbb{P}(f(Y_{n+1}|\mathbf{x}_{n+1}) \ge t|\mathbf{x}_{n+1})\\ &= \mathbb{P}(U_{n+1} \ge t|\mathbf{x}_{n+1}),\end{aligned}$$

where the next-to-last equality follows from the definition of the profile of the density.

For every $K \in \mathbb{R}$, let $Q(K) := \left|\{i : f(Y_i|\mathbf{x}_i) \ge K\}\right|$. Because U_i's are conditionally independent and identically distributed, then $Q(K)|W \sim \text{Binomial}(m, \mathbb{P}(f(Y_1|\mathbf{x}_1) \ge K))$. It follows that $Q(K)/m \xrightarrow[a.s.]{m \longrightarrow \infty} \mathbb{P}(f(Y_1|\mathbf{x}_1) \ge K)$. In particular, $Q(t^*)/m \xrightarrow[a.s.]{m\longrightarrow\infty} 1-\alpha$. Now, by definition $Q(T_m)/m \xrightarrow[a.s.]{m\longrightarrow\infty} 1-\alpha$. Conclude that $T_m \xrightarrow[a.s.]{m\longrightarrow\infty} t^*$.

□

Proof of Theorem 3.9. Item (i) was already shown as part of the proof of Theorem 3.8. To show (ii), assume that $t^*(\mathbf{x}_a,\alpha) = t^*(\mathbf{x}_b,\alpha)$ for every $\alpha \in (0,1)$. Now, notice that $t^*(\mathbf{x}_a,\alpha)$ is such that $g_{\mathbf{x}_a}(t^*(\mathbf{x}_a,\alpha)) = 1-\alpha$. Conclude that $g_{\mathbf{x}_a}(t^*(\mathbf{x}_a,\alpha)) = g_{\mathbf{x}_b}(t^*(\mathbf{x}_b,\alpha))$ for every $\alpha \in (0,1)$. Now, because $\widehat{f}$ is continuous, $\{t^*(\mathbf{x}_a,\alpha) : \alpha \in (0,1)\} = \text{Im}(\widehat{f}(\cdot|\mathbf{x}_a))$. Thus, $g_{\mathbf{x}_a} = g_{\mathbf{x}_b}$, and therefore $\mathbf{x}_a \sim \mathbf{x}_b$. □