# 368 A Appendix

#### 369 A.1 Additional theoretical results and proofs

- <sup>370</sup> We first prove an auxiliary Lemma.
- **Lemma 2.** For any  $\tau, \tau' \in [0, 1]$  with  $\tau < \tau'$  and cumulative distribution function F with inverse
- $F^{-1}$ , let  $t \equiv F^{-1}(\tau)$  and  $t' \equiv F^{-1}(\tau')$  and consider the scaled and vertically shifted Heaviside step
- 373 function  $H_{\theta}^{\tau,\tau'}(z) \equiv \tau + (\tau' \tau) \mathbb{1}_{z \geq \theta}$ . Then, for any  $p \in \mathbb{R}, p > 1$ , the set of  $\theta \in [t, t']$  minimizing

$$\int_{t}^{t'} |F(z) - H_{\theta}^{\tau,\tau'}|^{p} dz$$
(15)

374 is given by

$$\left\{\theta \in [t, t'] | F(\theta) = \left(\frac{\tau + \tau'}{2}\right)\right\}.$$
(16)

In particular, if  $F^{-1}$  is the inverse CDF, then  $F^{-1}((\tau + \tau')/2)$  is always a valid minimizer, and if  $F^{-1}$  is continuous at  $(\tau + \tau')/2$ , then  $F^{-1}((\tau + \tau')/2)$  is the unique minimizer.

377 Proof. We decompose the integral as follows

$$\int_{t}^{t'} |F(z) - H_{\theta}^{\tau,\tau'}(z)|^{p} dz = \int_{t}^{\theta} (F(z) - \tau)^{p} dz + \int_{\theta}^{t'} (\tau' - F(z))^{p} dz$$
(17)

$$= \lim_{a \to t} \int (F(z) - \tau)^p dz \Big|_a^\theta + \lim_{b \to t'} \int (\tau' - F(z))^p dz \Big|_\theta^b$$
(18)

where the limits are taken to cover the particular cases of  $t = -\infty$  and  $t' = \infty$ . Since we are minimizing with respect to  $\theta$  we can drop the constant terms and consider

$$\frac{d}{d\theta} \int (F(z) - \tau)^p dz|_{\theta} - \int (\tau' - F(z))^p dz|_{\theta} = (F(\theta) - \tau)^p - (\tau' - F(\theta))^p.$$
(19)

First note that for  $\theta \in [t, t']$ , we have  $F(\theta) - \tau > 0$  and  $\tau' - F(\theta) > 0$ . Then, equating the derivative to zero yields

$$(F(\theta) - \tau)^p - (\tau' - F(\theta))^p = 0$$
(20)

$$\Leftrightarrow F(\theta) - \tau = \tau' - F(\theta) \tag{21}$$

$$\Rightarrow F(\theta) = \frac{\tau + \tau'}{2}.$$
(22)

By replacing = by < in the previous equations, we see that the sign of the derivative is negative for  $\theta < F^{-1}(\frac{\tau+\tau'}{2})$  (since F is increasing) and positive otherwise, which proves the claim.

¢

**Theorem 1.** Given  $p_i \ge 0, i = 1..N$  such that  $\sum_i p_i = 1$ , the  $\ell_p$  distance between F and a mixture of Heaviside step functions  $F_N(z) = \sum_{i=1}^N p_i \mathbb{1}_{z \ge \theta_i}$  is minimized with  $\theta_i = F^{-1}((\tau_i + \tau_{i-1})/2)$ where  $\tau_i$  are the quantile levels  $\tau_i = \sum_{j=1}^i p_j$ .

*Proof.* Let  $t_i \equiv F^{-1}(\tau_i)$ . We first prove that an optimal  $\theta^*$  satisfies  $t_{i-1} \leq \theta_i^* \leq t_i$ . See Fig. 8 for an intuition.

Without loss of generality, we assume that  $\theta_1^* \leq \ldots \leq \theta_N^*$ . Let us suppose that there is an optimal  $F_N$  with  $\theta_1 \geq t_1$ . We can write the *p*-th power of the  $\ell_p$  distance as

$$\ell_p^p(F, F_N) = \int_{-\infty}^{t_1} |F(z) - F_N(z)|^p dz + \int_{t_1}^{\theta_2} |F(z) - F_N(z)|^p dz + \int_{\theta_2}^{\infty} |F(z) - F_N(z)|^p dz$$
(23)

The value of the middle term strictly decreases when  $\theta_1$  decreases toward  $t_1$  (while the other terms are unaffected) since

$$\int_{t_1}^{\theta_2} |F(z) - F_N(z)|^p dz = \int_{t_1}^{\theta_2} |F(z) - H_{\theta_1}^{0,\tau_1}(z)|^p dz$$
(24)

$$= \int_{t_1}^{\theta_1} F(z)^p dz + \int_{\theta_1}^{\theta_2} (F(z) - \tau_1)^p dz$$
(25)



Figure 8: Intuition for proving  $t_{i-1} \le \theta_i^* \le t_i$ . The  $\ell_p$  distance can be decreased by moving  $\theta_n$  in the first situation and  $\theta_{n+1}$  to  $t_n$  in the second one. The shaded area represents the improvement for p = 1.

- and  $F(z)^p > (F(z) \tau_1)^p$ . In consequence  $\theta_1 = t_1$ ; It proves that no optimal exist for  $\theta_1 > t_1$ , and thus that we have  $\theta_1 \le t_1$ .
- By induction, we assume that  $\theta_{n-1}^* \leq t_{n-1}$ . As before, we suppose, that there is an optimal  $F_N$  with  $\theta_n \geq t_n$  and we observe that the value of the term

$$\int_{t_n}^{\theta_{n+1}} |F(z) - F_N(z)|^p dz = \int_{t_n}^{\theta_{n+1}} |F(z) - H_{\theta_n}^{\tau_{n-1},\tau_n}(z)|^p dz$$
(26)

$$= \int_{t_n}^{\theta_n} (F(z) - \tau_{n-1})^p dz + \int_{\theta_n}^{\theta_{n+1}} (F(z) - \tau_n)^p dz \qquad (27)$$

strictly decreases when  $\theta_n$  decreases toward  $t_n$  since  $(F(z) - \tau_{n-1})^p > (F(z) - \tau_n)^p$ . In consequence  $\theta_n = t_n$ ; It proves that no optimal exist for  $\theta_n > t_n$ , and thus that we have  $\theta_n \le t_n \forall n \in \{1..N\}$ .

(starting by  $\theta_N$  and going backwards). This allows us to show that the optimization problem has an optimal substructure and thus it amounts to solving independent minimization problems of the form (15) i.e.

$$\min_{\theta_1,\dots,\theta_N} \ell_p^p(F,F_N) = \min_{\theta_1,\dots,\theta_N} \sum_{i=1}^N \int_{t_{i-1}}^{t_i} |F(z) - F_N(z)|^p dz$$
(28)

$$=\sum_{i=1}^{N}\min_{\theta_{i}}\int_{t_{i-1}}^{t_{i}}|F(z)-H_{\theta_{i}}^{\tau_{i-1},\tau_{i}}(z)|^{p}dz$$
(29)

402 with  $t_0 \equiv -\infty$ .

**Lemma 1.** Given two staircase distributions  $F(z) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{z \ge \theta_i}$  and  $\overline{F}(z) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{z \ge \overline{\theta}_i}$ such that  $\theta_1 < \cdots < \theta_N$  and  $\overline{\theta}_1 < \cdots < \overline{\theta}_N$ . Let  $u_{ij} \equiv \overline{\theta}_j - \theta_i$  and  $\delta_{ij} \equiv \mathbb{1}_{u_{ij} < 0}$ . The squared *Cramér distance between the distributions can be expressed as* 

$$\int_{-\infty}^{\infty} (F(z) - \bar{F}(z))^2 dz = \frac{1}{N^2} \sum_{i=1}^{N} |u_{ii}| + 2 \left( \sum_{j=i+1}^{N} \delta_{ij} |u_{ij}| + \sum_{j=1}^{i-1} (1 - \delta_{ij}) |u_{ij}| \right).$$
(11)



Figure 9: Computing the Cramér distance between  $\overline{F}$  (red) and F (blue) with a tiling operator. a) starting point represents  $\rho_1 = \frac{1}{N^2} \sum_{r \in R_1} u_r$ . b) ending point represents the squared Cramér distance  $\frac{1}{N^2} (u_1 1^2 + u_2 2^2 + u_3 3^2)$ , where  $u_i$  is the width of each rectangles in b). Notice that only the leftmost part of the leftmost rectangle of a) remains in b), the rest has been replaced by taller rectangles occupying the whole height. The middle diagram illustrates the effect of the tiling operator  $\rho_2$  yielding the final rectangle in the middle and, on the right, two overlapping rectangles—that need to be replaced by a taller one—and an oversubstracted rectangle in pink. The result of  $\rho_1 + \rho_2 + \rho_3$ is shown in b), a rectangle of height 3 has been added, the two overlapping rectangles have been removed and the pink rectangle has been added back.

*Proof.* In order to compute the squared Cramér distance on a uniform grid, we proceed in a constructive way as follows. The idea is to cover the area between the two curves with rectangular tiles as in Fig. 9 to compute the integral by pieces. A tile of height i/N and width u corresponds to the term  $u(i/N)^2$ . We start from Fig. 9 a) and replace parts of tiles to arrive to b).

Our demonstration unfold through these steps; First, we prove formally that our operator is well built: the sum of the tiling measured with the operator  $\rho$  is equal to the Cramér distance between the two curves. Secondly, we derive Eq. (11) by using that tiling operator.

First consider an interval  $u^+ \equiv [t_1, t_2]$  such that  $\overline{F}(t_1) = F(t_1)$ ,  $\overline{F}(t_2) = F(t_2)$  and  $\overline{F}(z) > F(z) \quad \forall z \in (t_1, t_2)$ . Let us define the tiling operator  $\rho_h$  for  $h \ge 1$ 

$$\rho_h(F,\bar{F},u^+) \equiv \sum_{r \in R_h} u_r \left(\frac{h}{N}\right)^2 - 2u_r \left(\frac{h-1}{N}\right)^2 + \mathbb{1}_{h>1} u_r \left(\frac{h-2}{N}\right)^2 \tag{30}$$

$$= \begin{cases} \sum_{r \in R_h} \frac{u_r}{N^2}, & \text{for } h = 1\\ \sum_{r \in R_h} \frac{2u_r}{N^2}, & \text{otherwise} \end{cases}$$
(31)

where  $u_r$  is the width of a rectangle r in the set  $R_h$  of rectangles of height h whose upper left and lower right angles are aligned with quantiles of, respectively,  $\overline{F}$  and F lying in  $u^+$ . Note that these rectangles lie completely within the difference area since F and  $\overline{F}$  are monotonically increasing. Note that  $\rho_1$  corresponds to the initial step depicted in Fig. 9 a). Intuitively, for h > 1, the operator replaces parts of width  $u_r$  of two tiles of height h - 1 by a tile of height h and width  $u_r$  and fixes oversubstracted tiles of the step h - 2.

More formally, let us define  $\rho^h(F, \overline{F}, u^+) \equiv \sum_{d=1}^h \rho_d(F, \overline{F}, u^+)$ . We prove by induction the following property. Given a partition of  $u^+$  in a set of intervals  $U^+$  such that for any  $u \in U^+$ ,

$$\bar{F}(z) - F(z) = \frac{d_u}{N} > 0 \ \forall z \in u,$$
(32)

423 where  $d_u$  depends on u only, then

$$\rho^{h}(F,\bar{F},u^{+}) = \frac{1}{N^{2}} \sum_{u \in U^{+}} |u| \left[ \mathbb{1}_{d_{u} \le h} d_{u}^{2} + \mathbb{1}_{d_{u} > h} \left[ (d_{u} - h + 1)h^{2} - (d_{u} - h)(h - 1)^{2} \right] \right].$$
(33)

For h = 1, in any interval u, there are  $d_u$  tiles of height 1 that have a non-empty projection on utherefore

$$\rho^{h}(F,\bar{F},u^{+}) = \frac{1}{N^{2}} \sum_{u \in U^{+}} |u| d_{u}$$
(34)

since  $\mathbb{1}_{d_u \leq h} d_u^2 + \mathbb{1}_{d_u > h} (d_u - h + 1)h^2 = d_u$ , which validates the base case.

For h > 1, for each  $r \in \mathbb{R}_h$ ,  $\rho_h$  adds three terms that can be decomposed in terms that match the segments of  $U^+$ . By noting that for each interval  $u \in U^+$  there will be  $\mathbb{1}_{d_u \ge h}(d_u - h + 1)$  rectangles in  $R_h$  with non-empty projection on u, we have

$$\rho_h(F,\bar{F},u^+) = \frac{1}{N^2} \sum_{u \in U^+} |u| \mathbb{1}_{d_u \ge h} (d_u - h + 1) \left[ h^2 - 2(h-1)^2 + (h-2)^2 \right]$$
(35)

Assuming the property holds for h - 1, we have

$$\rho^h(F,\bar{F},u^+) \tag{36}$$

$$=\rho^{h-1}(F,\bar{F},u^{+}) + \rho_{h}(F,\bar{F},u^{+})$$
(37)

$$= \frac{1}{N^2} \sum_{u \in U^+} |u| \left( \mathbb{1}_{d_u \le h-1} d_u^2 + \mathbb{1}_{d_u > h-1} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 2)(h-1)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right] + \frac{1}{N^2} \left[ (d_u - h + 1)(h-2)^2 - (d_u - h + 1)(h-2)^2 \right]$$

$$\mathbb{1}_{d_u \ge h} (d_u - h + 1) \left[ h^2 - 2(h - 1)^2 + (h - 2)^2 \right]$$
(38)

$$= \frac{1}{N^2} \sum_{u \in U^+} |u| \left( \mathbb{1}_{d_u \le h-1} d_u^2 + \mathbb{1}_{d_u \ge h} \left[ (d_u - h + 1)h^2 - (d_u - h)(h - 1)^2 \right] \right)$$
(39)

$$= \frac{1}{N^2} \sum_{u \in U^+} |u| \left( \mathbb{1}_{d_u \le h} d_u^2 + \mathbb{1}_{d_u > h} \left[ (d_u - h + 1)h^2 - (d_u - h)(h - 1)^2 \right] \right)$$
(40)

431 since  $\mathbb{1}_{d_u > h-1} = \mathbb{1}_{d_u \ge h}$  and  $\mathbb{1}_{d_u = h} \left[ (d_u - h + 1)h^2 - (d_u - h)(h - 1)^2 \right] = \mathbb{1}_{d_u = h} d_u^2$ .

Since  $\mathbb{1}_{d_u \leq N} = 1 - \mathbb{1}_{d_u > N} = 1$ , the final tiling  $\rho^N(F, \overline{F}, u^+)$  corresponds to the Cramér distance on the interval  $u^+$ , i.e.

$$\rho^{N}(F,\bar{F},u^{+}) = \frac{1}{N^{2}} \sum_{u \in U^{+}} |u| d_{u}^{2}.$$
(41)

Now, we are going to use (31) to get to the claimed expression. First note that for a rectangle  $r \in R_h$ with upper leftmost and lower rightmost angles corresponding, respectively, to  $\bar{\theta}_j$  and  $\theta_i$ , its width is  $u_r = |u_{ij}|$ . Since  $\theta_1 < \cdots < \theta_N$  and  $\bar{\theta}_1 < \cdots < \bar{\theta}_N$ , the condition that  $\bar{F}(z) > F(z)$  for such rectangles is equivalent to  $\delta_{ij} = 1 \land i \leq j$ . By symmetry,  $\bar{F}(z) < F(z)$  is equivalent to  $\delta_{ij} = 0 \land j \leq i$ . We consider the case i = j separately to avoid double counting and also because it corresponds to h = 1. Therefore, from (31), we have

$$\rho^{N}(F,\bar{F},\mathbb{R}) = \sum_{r \in R_{1}} \frac{u_{r}}{N^{2}} + \sum_{h=2}^{N} \sum_{r \in R_{h}} \frac{2u_{r}}{N^{2}}$$
(42)

$$=\sum_{i=1}^{N} \frac{|u_{ii}|}{N^2} + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \delta_{ij} \frac{2|u_{ij}|}{N^2} + \sum_{j=1}^{N-1} \sum_{i=j+1}^{N} (1-\delta_{ij}) \frac{2|u_{ij}|}{N^2}.$$
 (43)

By taking out common factors and swapping the indices of the two rightmost sums, we get the expression (11).  $\Box$ 

442 **Corollary 2.** For  $F(z) \equiv \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{z \ge \theta_i}$  and  $\bar{F}(z) \equiv \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{z \ge \bar{\theta}_i}$  we have

$$\frac{\partial \mathcal{L}_{QR}(F,\bar{F})}{\partial \theta_i} = \frac{1}{N} \left( \frac{1-2i}{2} + \sum_{j=1}^N \delta_{ij} \right) \text{ and } \frac{\partial \ell_2^2(F,\bar{F})}{\partial \theta_i} = \frac{1}{N^2} \left( 1 - 2i + 2\sum_{j=1}^N \delta_{ij} \right)$$
(12)

443 where  $\delta_{ij} \equiv \mathbb{1}_{u_{ij} < 0}$ . Therefore, their gradients are collinear, i.e.

$$\nabla_{\theta} \mathcal{L}_{\text{QR}} = \frac{N}{2} \nabla_{\theta} \ell_2^2. \tag{13}$$

444 *Proof.* For a target distribution  $\bar{F}(z) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{z \ge \bar{\theta}_i}$ , the quantile regression loss can be expressed 445 as

$$\mathcal{L}_{QR}(F,\bar{F}) = \sum_{i=1}^{N} \frac{1}{N} \sum_{j=1}^{N} \rho_{\hat{\tau}_i}(\bar{\theta}_j - \theta_i)$$
(44)

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} (\bar{\theta}_j - \theta_i) (\hat{\tau}_i - \delta_{ij})$$
(45)

446 and thus

$$\frac{\partial \mathcal{L}_{QR}(F,\bar{F})}{\partial \theta_i} = \frac{1}{N} \sum_{j=1}^N (\delta_{ij} - \hat{\tau}_i)$$
(46)

$$= \frac{1}{N} \left( \frac{1-2i}{2} + \sum_{j=1}^{N} \delta_{ij} \right).$$
 (47)

In order to obtain the partial derivative of the squared Cramér distance, first note that  $\delta_{ij}|u_{ij}| = \delta_{ij}(\theta_i - \bar{\theta}_j), (1 - \delta_{ij})|u_{ij}| = (1 - \delta_{ij})(\bar{\theta}_j - \theta_i)$  and  $|u_{ii}| = \delta_{ii}(\theta_i - \bar{\theta}_i) + (1 - \delta_{ii})(\bar{\theta}_i - \theta_i)$ . By replacing these quantities in (11) and taking the derivative with respect to  $\theta_i$  we obtain

$$\frac{\partial \ell_2^2(F,\bar{F})}{\partial \theta_i} = \frac{1}{N^2} \left[ 2\delta_{ii} - 1 + 2\left(\sum_{j=i+1}^N \delta_{ij} + \sum_{j=1}^{i-1} (\delta_{ij} - 1)\right) \right]$$
(48)

$$= \frac{1}{N^2} \left( 2\sum_{j=1}^N \delta_{ij} - 1 + 2\sum_{j=1}^{i-1} (-1) \right)$$
(49)

$$= \frac{1}{N^2} \left( 1 - 2i + 2\sum_{j=1}^N \delta_{ij} \right).$$
 (50)

450

### 451 A.2 Correctness of Algorithm 1

**Proposition 1.** Given two distributions  $F(z) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{z \ge \theta_i}$ , and  $\bar{F}(z) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{z \ge \bar{\theta}_i}$ , Algorithm 1 computes

$$\int_{-\infty}^{\infty} (F(z) - \bar{F}(z))^2 dz = \sum_{i=1}^{2N-1} \left( \theta'_{i+1} - \theta'_i \right) \left( \sum_{j \text{ s.t. } \theta_j \le \theta'_i} \frac{1}{N} - \sum_{j \text{ s.t. } \bar{\theta}_j \le \theta'_i} \frac{1}{N} \right)^2.$$
(51)

454 *Proof.* Consider the sorted sequence of merged quantiles

$$\boldsymbol{\theta}' \equiv \theta_1', \dots, \theta_{2N}' \equiv \operatorname{sort}\left(\{\theta_i\}_{i=1..N} \bigcup \{\bar{\theta}_i\}_{i=1..N}\right).$$
(52)

455 We have that  $F(z) - \bar{F}(z) \equiv \Delta_i$  is constant in  $[\theta'_i, \theta'_{i+1}), \forall i \in 1..2N$ . Therefore,

$$\int_{-\infty}^{\infty} (F(z) - \bar{F}(z))^2 dz = \sum_{i=1}^{2N-1} \int_{\theta'_i}^{\theta'_{i+1}} (F(z) - \bar{F}(z))^2 dz = \sum_{i=1}^{2N-1} (\theta'_{i+1} - \theta'_i) \Delta_i$$
(53)

456 If  $\theta'_i \leq z < \theta'_{i+1}$ , then

$$F(z) = \frac{1}{N} \sum_{j=1}^{N} \mathbb{1}_{z \ge \theta_j} = \frac{1}{N} \sum_{j \text{ s.t. } \theta_j \le \theta'_i} 1$$
(54)

$$\bar{F}(z) = \frac{1}{N} \sum_{j=1}^{N} \mathbb{1}_{z \ge \bar{\theta}_j} = \frac{1}{N} \sum_{j \text{ s.t. } \bar{\theta}_j \le \theta'_i} 1$$
(55)

457 and thus

$$\Delta_{i} = \sum_{j \text{ s.t. } \theta_{j} \le \theta'_{i}} \frac{1}{N} - \sum_{j \text{ s.t. } \bar{\theta}_{j} \le \theta'_{i}} \frac{1}{N},$$
(56)

458 which proves (51).

The algorithm computes the differences  $(\theta'_{i+1} - \theta'_i)$  and stores them in  $\Delta_z$ . After the steps

$$\Delta_{\tau} \leftarrow \operatorname{concat}\left(-\frac{1}{N}\mathbf{1}_{N}, \frac{1}{N}\mathbf{1}_{N}\right)$$
(57)

$$\Delta_{\tau} \leftarrow \Delta_{\tau}[i_1, \dots, i_N], \tag{58}$$

in words, the *i*-th element of the vector  $\Delta_{\tau}$  is -1 if  $\theta'_i$  comes from  $\overline{\theta}$  and 1 otherwise, i.e.

$$\Delta_{\tau}[i] = (-1)^{\mathbb{I}_{\exists j \theta'_i \equiv \bar{\theta}_j}}$$
<sup>(59)</sup>

<sup>461</sup> where  $\equiv$  denotes symbol equality. After the final step

$$\Delta_{\tau} \leftarrow \operatorname{cumsum}\left(\Delta_{\tau}\right) [: -1],\tag{60}$$

the *i*-th element of the vector  $\Delta_{\tau}$  can be expressed as

$$\Delta_{\tau}[i] = \frac{1}{N} \sum_{k=1}^{i} (-1)^{\mathbb{1}_{\exists j \, \theta'_k \equiv \bar{\theta}_j}}.$$
(61)

If  $\theta'_i \neq \theta'_{i+1}$ , then  $\Delta_{\tau}[i] = \Delta_i$ . Otherwise,  $\Delta_{\tau}[i] \neq \Delta_i$ , but, since  $\theta'_{i+1} - \theta'_i = 0$ , the corresponding term in (51) is zero too. Therefore, the algorithm produces the claimed output.

## 465 A.3 Hyperparameters

All the experimental results for CNC-CR-DQN, NC-CR-DQN and CR-DQN were obtained with the hyperparameters' values shown in Table 1, which are the same that those used to generate the QR-DQN results provided by DQN\_ZOO. The last two hyperparameters are specific to CNC-QR-DQN and NC-CR-DQN.

#### 470 A.4 Additional experimental results

Fig. 10 shows the online training performance of CNC-CR-DQN in comparison to the pure distributional contenders C51, QR-DQN and IQN, on the full Atari-57 benchmark.



Figure 10: **Training performance on the Atari-57 benchmark.** Curves are averages over a number of seeds, smoothed over a sliding window of 5 iterations, and error bands give standard deviations. For C51, QR-DQN and IQN, 5 seeds were used (provided by DQN\_Z00 [24]). For CNC-CR-DQN, 3 seeds were used for all the games except those indicated by \*, for which only 2 seeds were used.

Hyperparameter	Value	Comment
replay_capacity	1e6	
min_replay_capacity_fraction	0.05	Min replay set size for learning
batch_size	32	
max_frames_per_episode	108000	= 30 min
num_action_repeats	4	In frames
num_stacked_frames	4	
exploration_epsilon_begin_value	1	
exploration_epsilon_end_value	0.01	
exploration_epsilon_decay_frame_fraction	0.02	
eval_exploration_epsilon	0.001	
target_network_update_period	4e4	
learning_rate	5e-5	
optimizer_epsilon	0.01 / 32	ADAM's parameter
additional_discount	0.99	Discount_rate multiplier
max_abs_reward	1	
max_global_grad_norm	10	
num_iterations	200	
num_train_frames	1e6	Per iteration
num_eval_frames	5e5	Per iteration
learn_period	16	One learning step each 16 frames
num_quantiles	201	N
Convolutional layer 1	32, (8, 8), (4, 4)	num_features, kernel_shape, stride
Convolutional layer 2	64, (4, 4), (2, 2)	-
Convolutional layer 3	64, (3, 3), (1, 1)	
n_layers	1	Number of hidden layers $\lambda$
n_nodes	512	Number of nodes $\eta$ per hidden layer

# Table 1: Hyperparameters used in our DQN\_ZOO implementation of CNC-CR-DQN.