# On the Relationship Between Binary Classification, Bipartite Ranking, and Binary Class Probability Estimation

## Appendix

## A Proof of Theorem 4

*Proof.* Assume w.l.o.g. that $\text{Thresh}_{D,f,c}(u) = \text{sign}(u - t^*)$ for some $t^* \in [-\infty, \infty]$; a similar analysis can be shown when $\text{Thresh}_{D,f,c}(u) = \overline{\text{sign}}(u - t^*)$ for some $t^*$. We first recall the following result of Clémençon et al. [8] (adapted as in [26] to account for ties and conditioning on $y \neq y'$).

$$\text{regret}_D^{\text{rank}}[f] = \frac{1}{2p(1-p)} \mathbf{E}_{x,x'}\Big[\big|\eta(x) - \eta(x')\big|\Big(\mathbf{1}\big((f(x) - f(x'))(\eta(x) - \eta(x')) < 0\big) + \frac{1}{2}\mathbf{1}\big(f(x) = f(x')\big)\Big)\Big].$$

Next, given a binary classifier $h : X \to \{\pm 1\}$ and a cost parameter $c \in (0,1)$, the cost-sensitive classification error can be rewritten as

$$\text{er}_D^{0\text{-}1,c}[h] = \mathbf{E}_x\big[(1-c)\eta(x)\mathbf{1}\big(h(x) = -1\big) + c\big(1 - \eta(x)\big)\mathbf{1}\big(h(x) = 1\big)\big]$$

and the corresponding regret can be expanded as

$$\begin{aligned}
&\text{regret}_D^{0\text{-}1,c}[h] \\
&= \mathbf{E}_x\big[(1-c)\eta(x)\mathbf{1}\big(h(x) = -1\big) + c\big(1 - \eta(x)\big)\mathbf{1}\big(h(x) = 1\big)\big] \\
&\qquad - \mathbf{E}_x\big[(1-c)\eta(x)\mathbf{1}\big(\eta(x) \le c\big) + c\big(1 - \eta(x)\big)\mathbf{1}\big(\eta(x) > c\big)\big] \\
&= \mathbf{E}_x\big[\big(c - \eta(x)\big)\mathbf{1}\big(h(x) = 1,\ \eta(x) \le c\big)\big] + \mathbf{E}_x\big[\big(\eta(x) - c\big)\mathbf{1}\big(h(x) = -1,\ \eta(x) > c\big)\big].
\end{aligned}$$

For $h = \text{sign} \circ (f - t^*)$,

$$\begin{aligned}
&\text{regret}_D^{0\text{-}1,c}[\text{sign} \circ (f - t^*)] \\
&= \mathbf{E}_x\big[\big(c - \eta(x)\big)\mathbf{1}\big(f(x) > t^*,\ \eta(x) \le c\big)\big] + \mathbf{E}_x\big[\big(\eta(x) - c\big)\mathbf{1}\big(f(x) \le t^*,\ \eta(x) > c\big)\big] \qquad (1)\\
&= a + b \ \text{(say)}.
\end{aligned}$$

We then have

$$\begin{aligned}
2p(1-p)\ \text{regret}_D^{\text{rank}}[f] &\ge \frac{1}{2}\mathbf{E}_{x,x'}\Big[\big|\eta(x) - \eta(x')\big|\Big(\mathbf{1}\big((f(x) - f(x'))(\eta(x) - \eta(x')) \le 0\big)\Big)\Big] \\
&\qquad \text{(getting rid of the term accounting for ties)} \\
&\ge \frac{1}{2}\mathbf{E}_{x,x'}\Big[\big|\eta(x) - \eta(x')\big|\Big(\mathbf{1}\big(f(x) \ge f(x'),\ \eta(x) \le c,\ \eta(x') > c\big) \\
&\qquad + \mathbf{1}\big(f(x) \le f(x'),\ \eta(x) > c,\ \eta(x') \le c\big)\Big)\Big] \\
&= \frac{2}{2}\mathbf{E}_{x,x'}\Big[\big|\eta(x) - \eta(x')\big|\Big(\mathbf{1}\big(f(x) \ge f(x'),\ \eta(x) \le c,\ \eta(x') > c\big)\Big)\Big] \\
&= \text{term}_1 + \text{term}_2 + \text{term}_3, \qquad (2)
\end{aligned}$$

where

$$\begin{aligned}
\text{term}_1 &= \mathbf{E}_{x,x'}\Big[\big|\eta(x) - \eta(x')\big|\Big(\mathbf{1}\big(f(x) \ge f(x') > t^*,\ \eta(x) \le c,\ \eta(x') > c\big)\Big)\Big], \\
\text{term}_2 &= \mathbf{E}_{x,x'}\Big[\big|\eta(x) - \eta(x')\big|\Big(\mathbf{1}\big(t^* \ge f(x) \ge f(x'),\ \eta(x) \le c,\ \eta(x') > c\big)\Big)\Big] \quad \text{and} \\
\text{term}_3 &= \mathbf{E}_{x,x'}\Big[\big|\eta(x) - \eta(x')\big|\Big(\mathbf{1}\big(f(x) > t^*,\ f(x') \le t^*,\ \eta(x) \le c,\ \eta(x') > c\big)\Big)\Big].
\end{aligned}$$

Each of the above terms corresponds to different sets of pairs of instances; $\text{term}_1$ corresponds to pairs where both instances are ranked by $f$ above $t^*$; $\text{term}_2$ corresponds to pairs where both instances are ranked by $f$ below (or at the same position as) $t^*$; term$_3$ corresponds to pairs $(x, x')$, where $x$ is ranked by $f$ above $t^*$, while $x'$ is ranked below (or at the same position as) $t^*$. We next bound each of these terms separately.

term$_1$

$$
\begin{aligned}
&= \mathbf{E}_{x,x'}\Big[\big|\eta(x') - c + c - \eta(x)\big|\Big(\mathbf{1}\big(f(x) \geq f(x') > t^*,\ \eta(x) \leq c,\ \eta(x') > c\big)\Big)\Big] \\
&\geq \mathbf{E}_{x,x'}\Big[2\big|\eta(x') - c\big|\big|c - \eta(x)\big|\Big(\mathbf{1}\big(f(x) \geq f(x') > t^*,\ \eta(x) \leq c,\ \eta(x') > c\big)\Big)\Big] \\
&\qquad\qquad (\text{since } u + v \geq 2\sqrt{uv} \geq 2uv,\ \forall u, v \in [0,1]) \\
&= 2\mathbf{E}_x\Big[\big|c - \eta(x)\big|\mathbf{1}(f(x) > t^*,\ \eta(x) \leq c)\mathbf{E}_{x'}\big[\big|\eta(x') - c\big|\mathbf{1}\big(t^* < f(x') \leq f(x),\ \eta(x') > c\big)\big]\Big].
\end{aligned} \tag{3}
$$

By definition, $t^*$ yields the minimum classification regret among all choices of thresholds $t \in \mathbb{R}$:

$$
\begin{aligned}
t^* &= \operatorname*{argmin}_{t \in [-\infty,\infty]} \Big\{\text{regret}_D^{0\text{-}1,c}\big[\text{sign} \circ \big(f - t\big)\big]\Big\} \\
&= \operatorname*{argmin}_{t \in [-\infty,\infty]} \mathbf{E}_{x'}\big[\big(\eta(x') - c\big)\mathbf{1}\big(f(x') \leq t,\ \eta(x') > c\big) + \big(c - \eta(x')\big)\mathbf{1}\big(f(x') > t,\ \eta(x') \leq c\big)\big] \\
&\qquad\qquad (\text{from Eq. (1)}).
\end{aligned}
$$

It can hence be shown that for any $t > t^*$,

$\mathbf{E}_{x'}\big[\big|\eta(x') - c\big|\mathbf{1}\big(t^* < f(x') \leq t,\ \eta(x') > c\big)\big] \geq \mathbf{E}_{x'}\big[\big|c - \eta(x')\big|\mathbf{1}\big(t^* < f(x') \leq t,\ \eta(x') \leq c\big)\big]$.

Applying the above inequality to Eq. (3) with $t = f(x)$, we have

term$_1$

$$
\begin{aligned}
&\geq 2\mathbf{E}_x\Big[\big|c - \eta(x)\big|\mathbf{1}(f(x) > t^*,\ \eta(x) \leq c)\mathbf{E}_{x'}\big[\big|c - \eta(x')\big|\mathbf{1}\big(t^* < f(x') \leq f(x),\ \eta(x') \leq c\big)\big]\Big] \\
&\geq \frac{2}{2}\mathbf{E}_x\Big[\big|c - \eta(x)\big|\mathbf{1}(f(x) > t^*,\ \eta(x) \leq c)\mathbf{E}_{x'}\big[\big|c - \eta(x')\big|\mathbf{1}\big(t^* < f(x'),\ \eta(x') \leq c\big)\big]\Big] \\
&\qquad\qquad (\text{since } \mathbf{E}_{x,x'}[g(x,x')\mathbf{1}(f(x) \leq f(x'))] \geq \frac{1}{2}\mathbf{E}_{x,x'}[g(x,x')]) \\
&= \mathbf{E}_x\Big[\big|c - \eta(x)\big|\mathbf{1}(f(x) > t^*,\ \eta(x) \leq c)\Big]\mathbf{E}_{x'}\Big[\big|c - \eta(x')\big|\mathbf{1}\big(t^* < f(x'),\ \eta(x') \leq c\big)\Big] \\
&= \mathbf{E}_x\Big[\big|c - \eta(x)\big|\mathbf{1}(f(x) > t^*,\ \eta(x) \leq c)\Big]^2 \\
&= a^2.
\end{aligned}
$$

Similarly, one can show

$$
\text{term}_2 \quad \geq \quad \mathbf{E}_x\Big[\big|\eta(x) - c\big|\mathbf{1}(f(x) \leq t^*,\ \eta(x) > c)\Big]^2 \ = \ b^2.
$$

In the case of term$_3$, we have

$$
\begin{aligned}
\text{term}_3 &= \mathbf{E}_{x,x'}\Big[\big|\eta(x') - c + c - \eta(x)\big|\Big(\mathbf{1}\big(f(x) > t^*,\ f(x') \leq t^*,\ \eta(x) \leq c,\ \eta(x') > c\big)\Big)\Big] \\
&\geq \mathbf{E}_{x,x'}\Big[2\big|\eta(x') - c\big|\big|c - \eta(x)\big|\Big(\mathbf{1}\big(f(x) > t^*,\ f(x') \leq t^*,\ \eta(x) \leq c,\ \eta(x') > c\big)\Big)\Big] \\
&\qquad\qquad (\text{since } u + v \geq 2\sqrt{uv} \geq 2uv,\ \forall u, v \in [0,1]) \\
&\geq 2\mathbf{E}_{x,x'}\Big[\big|c - \eta(x)\big|\mathbf{1}\big(f(x) > t^*,\ \eta(x) \leq c\big)\big|\eta(x') - c\big|\mathbf{1}\big(f(x') \leq t^*,\ \eta(x') > c\big)\Big] \\
&= 2\mathbf{E}_x\Big[\big|c - \eta(x)\big|\mathbf{1}\big(f(x) > t^*,\ \eta(x) \leq c\big)\Big]\mathbf{E}_{x'}\Big[\big|\eta(x') - c\big|\mathbf{1}\big(f(x') \leq t^*,\ \eta(x') > c\big)\Big] \\
&= 2ab.
\end{aligned}
$$

Applying the bounds on term$_1$, term$_2$ and term$_3$ in Eq. (2), we have

$$
\begin{aligned}
2p(1-p)\ \text{regret}_D^{\text{rank}}[f] &\geq a^2 + b^2 + 2ab \\
&= (a+b)^2 \\
&= \big(\text{regret}_D^{0\text{-}1,c}[\text{sign} \circ (f - t^*)]\big)^2.
\end{aligned}
$$

Hence the proof. □

## B Proof of Theorem 6

*Proof.*

$$
\begin{aligned}
&\text{regret}_D^{0\text{-}1,c}[\text{sign} \circ (f - \widehat{t}_{S,f,c})] \\
&= \text{er}_D^{0\text{-}1,c}[\text{sign} \circ (f - \widehat{t}_{S,f,c})] - \text{er}_D^{0\text{-}1,c,*} \\
&= \text{er}_D^{0\text{-}1,c}[\text{sign} \circ (f - \widehat{t}_{S,f,c})] - \text{er}_D^{0\text{-}1,c}[\text{Thresh}_{D,f,c} \circ f] + \text{er}_D^{0\text{-}1,c}[\text{Thresh}_{D,f,c} \circ f] - \text{er}_D^{0\text{-}1,c,*} \\
&\qquad\qquad\qquad\qquad\qquad\qquad (\text{where Thresh}_{D,f,c} \text{ is obtained from (OP1)}) \\
&= \Big(\text{er}_D^{0\text{-}1,c}[\text{sign} \circ (f - \widehat{t}_{S,f,c})] - \text{er}_D^{0\text{-}1,c}[\text{Thresh}_{D,f,c} \circ f]\Big) + \text{regret}_D^{0\text{-}1,c}[\text{Thresh}_{D,f,c} \circ f].
\end{aligned} \tag{4}
$$

The second term in the above expression can be upper bounded in terms of the ranking regret of $f$ using Theorem 4. We now derive a bound on the first term by using standard VC-dimension based uniform convergence result for binary classification. Note that the real-valued function $f$, when applied to each instance drawn from $D$, induces a distribution over $\mathbb{R} \times \{\pm 1\}$; let us call this distribution $D_f$. Also, let $S_f = \{(f(x_1), y_1), \ldots, (f(x_n), y_n)\}$ be the set constructed by applying $f$ to each instance in $S$; given that $S$ is drawn iid from $D$, it follows that $S_f$ is also iid drawn from $D_f$. Recall that $\mathcal{T}_{\text{inc}}$ is the set of all increasing functions from $\mathbb{R}$ to $\{\pm 1\}$ (see Section 3). One can now view the optimization problem in (OP1) as risk minimization over $\mathcal{T}_{\text{inc}}$ w.r.t. the distribution $D_f$ and the optimization problem in (OP2) as empirical risk minimization over $\mathcal{T}_{\text{inc}}$ w.r.t. the training sample $S_f$. In other words,

$$
\inf_{\theta \in \mathcal{T}_{\text{inc}}} \Big\{ \text{er}_D^{0\text{-}1,c}\big[\theta \circ f\big] \Big\} = \inf_{\theta \in \mathcal{T}_{\text{inc}}} \Big\{ \text{er}_{D_f}^{0\text{-}1,c}\big[\theta\big] \Big\} = \text{er}_{D_f}^{0\text{-}1,c}\big[\theta^*\big]
$$

and

$$
\inf_{t \in \mathbb{R}} \Big\{ \text{er}_S^{0\text{-}1,c}\big[\text{sign} \circ \big(f - t\big)\big] \Big\} = \inf_{\theta \in \mathcal{T}_{\text{inc}}} \Big\{ \text{er}_{S_f}^{0\text{-}1,c}\big[\theta\big] \Big\} = \text{er}_{S_f}^{0\text{-}1,c}\big[\widehat{\theta}\big].
$$

Thus the first term in Eq. (4) evaluates to $\text{er}_{D_f}^{0\text{-}1,c}\big[\widehat{\theta}\big] - \text{er}_{D_f}^{0\text{-}1,c}\big[\theta^*\big]$. Using standard results, one can show that the following upper bound on this quantity holds with probability at least $1 - \delta$ (over the draw of $S \sim D^n$):

$$
\text{er}_{D_f}^{0\text{-}1,c}\big[\widehat{\theta}\big] - \text{er}_{D_f}^{0\text{-}1,c}\big[\theta^*\big] \le \sqrt{\frac{32\big(\text{VC-dim}(\mathcal{T}_{\text{inc}})\big(\ln(2n) + 1\big) + \ln\big(\frac{4}{\delta}\big)\big)}{n}},
$$

where VC-dim($\mathcal{T}_{\text{inc}}$) is the VC dimension of $\mathcal{T}_{\text{inc}}$. Thus with probability at least $1 - \delta$ (over the draw of $S \sim D^n$), we have

$$
\begin{aligned}
&\text{regret}_D^{0\text{-}1,c}[\text{sign} \circ (f - \widehat{t}_{S,f,c})] \\
&\le \sqrt{\frac{32\big(\text{VC-dim}(\mathcal{T}_{\text{inc}})\big(\ln(2n) + 1\big) + \ln\big(\frac{4}{\delta}\big)\big)}{n}} + \sqrt{2}\sqrt{p(1-p)\,\text{regret}_D^{\text{rank}}[f]}.
\end{aligned}
$$

It is easy to see that VC-dim($\mathcal{T}_{\text{inc}}$) $= 2$; plugging this in the above expression completes the proof. □

## C Proof of Theorem 10

Our proof for Theorem 10 is simpler than the one in [20] which holds for a more general result. We first state and prove two lemmas which will be useful in our proof.

**Lemma 20.** *Let $D$ be a distribution over $X \times \{\pm 1\}$. For any binary class probability estimator $\widehat{\eta} : X \to [0, 1]$ calibrated w.r.t. $D$ and threshold $t \in [0, 1]$,*

$$
\text{er}_D^{0\text{-}1,c}\big[\text{sign} \circ (\widehat{\eta} - t)\big] = \mathbf{E}_{s_{\widehat{\eta}}}\Big[(1-c)s_{\widehat{\eta}}\mathbf{1}(s_{\widehat{\eta}} \le t) + c\big(1 - s_{\widehat{\eta}}\big)\mathbf{1}(s_{\widehat{\eta}} > t)\Big]
$$

*and*

$$
\text{er}_D^{0\text{-}1,c}\big[\overline{\text{sign}} \circ (\widehat{\eta} - t)\big] = \mathbf{E}_{s_{\widehat{\eta}}}\Big[(1-c)s_{\widehat{\eta}}\mathbf{1}(s_{\widehat{\eta}} < t) + c\big(1 - s_{\widehat{\eta}}\big)\mathbf{1}(s_{\widehat{\eta}} \ge t)\Big],
$$

*where $s_{\widehat{\eta}}$ is the random variable associated with the score distribution of $\widehat{\eta}$ over $[0, 1]$.*

*Proof.* We give a proof for the first part of the result; the second part involving $\overline{\text{sign}}$ can be proved in a similar manner. For simplicity of notation, we omit the subscript on $s_{\widehat{\eta}}$. For any $c \in (0,1)$, we have

$$\begin{aligned}
&\text{er}_D^{\text{0-1},c}\big[\text{sign} \circ (\widehat{\eta} - t)\big] \\
&\quad= \mathbf{E}_x\big[(1-c)\eta(x)\mathbf{1}(\widehat{\eta}(x) \le t) \;+\; c\big(1-\eta(x)\big)\mathbf{1}(\widehat{\eta}(x) > t)\big] \\
&\quad= \mathbf{E}_s\Big[\mathbf{E}_x\big[(1-c)\eta(x)\mathbf{1}(\widehat{\eta}(x) \le t) \;+\; c\big(1-\eta(x)\big)\mathbf{1}(\widehat{\eta}(x) > t) \;\big|\; \widehat{\eta}(x) = s\big]\Big] \\
&\quad= \mathbf{E}_s\Big[(1-c)\mathbf{E}_x\big[\eta(x) \;\big|\; \widehat{\eta}(x) = s\big]\mathbf{1}(s \le t) \;+\; c\big(1 - \mathbf{E}_x\big[\eta(x) \;\big|\; \widehat{\eta}(x) = s\big]\big)\mathbf{1}(s > t)\big]\Big] \\
&\quad= \mathbf{E}_s\big[(1-c)\mathbf{P}(y=1|s)\mathbf{1}(s \le t) + c\big(1 - \mathbf{P}(y=1|s)\big)\mathbf{1}(s > t)\big] \\
&\qquad\qquad\qquad\qquad\text{(follows from } \mathbf{E}_x\big[\eta(x) \;\big|\; \widehat{\eta}(x) = s\big] = \mathbf{P}(y=1|s)\text{)}.
\end{aligned}$$

□

The next lemma states that for any binary class probability estimator $\widehat{\eta}$ calibrated w.r.t. $D$ and a given cost parameter $c \in (0,1)$, the optimal classification transform on $\widehat{\eta}$ that yields minimum cost-sensitive classification error is simply $\theta(u) = \text{sign}(u - c)$.

**Lemma 21.** *Let $D$ be a distribution over $X \times \{\pm 1\}$. For any binary class probability estimator $\widehat{\eta} : X \to [0,1]$ calibrated w.r.t. $D$ and cost parameter $c \in (0,1)$,*

$$\text{Thresh}_{D,\widehat{\eta},c} = \text{sign} \circ (\widehat{\eta} - c).$$

*Proof.* Let $s_{\widehat{\eta}}$ denote the random variable associated with the score distribution of $\widehat{\eta}$ over $[0,1]$; for simplicity of notation, we omit the subscript on $s_{\widehat{\eta}}$. Let us start by considering functions $\theta \in \mathcal{T}_{\text{inc}}$ of the form $\theta(u) = \text{sign}(u - t)$ for some $t \in [0,1]$. For any $c \in (0,1)$, we have

$$\begin{aligned}
&\text{argmin}_{t \in [0,1]}\Big\{\text{er}_D^{\text{0-1},c}\big[\text{sign} \circ (\widehat{\eta} - t)\big]\Big\} \\
&\quad= \text{argmin}_{t \in [0,1]}\Big\{\mathbf{E}_s\big[\underbrace{(1-c)s\mathbf{1}(s \le t) + c\big(1-s\big)\mathbf{1}(s > t)}_{\text{minimum at } t = c}\big]\Big\} \quad \text{(from Lemma 20)} \\
&\quad= c.
\end{aligned}$$

The last step follows from the fact that the point-wise minimum is attained at $t = c$; this implies that $\theta(u) = \text{sign}(u - c)$ yields the least possible value of $\text{er}_D^{\text{0-1},c}\big[\theta \circ \widehat{\eta}\big]$ over all increasing functions in $\mathcal{T}_{\text{inc}}$, and hence we have $\text{Thresh}_{D,\widehat{\eta},c} = \text{sign} \circ (\widehat{\eta} - c)$. □

We are now ready to prove Theorem 10. As before, let $s_{\widehat{\eta}}$ denote the random variable associated with the score distribution of $\widehat{\eta}$ over $[0,1]$; for simplicity of notation, let us omit the subscript on $s_{\widehat{\eta}}$.

*Proof of Theorem 10.* Starting with the right hand side, we have

$$\begin{aligned}
&2\mathbf{E}_{c \sim U(0,1)}\big[\text{er}_D^{\text{0-1},c}\big[\text{Thresh}_{D,f,c} \circ f\big]\big] \\
&\quad= 2\mathbf{E}_{c \sim U(0,1)}\big[\text{er}_D^{\text{0-1},c}\big[\text{sign} \circ (\widehat{\eta} - c)\big]\big] \quad \text{(from Lemma 21)} \\
&\quad= 2\mathbf{E}_{c \sim U(0,1)}\Big[\mathbf{E}_s\big[(1-c)s\mathbf{1}(s \le c) + c(1-s)\mathbf{1}(s > c)\big]\Big] \quad \text{(from Lemma 20)} \\
&\quad= 2\mathbf{E}_s\Big[\mathbf{E}_{c \sim U(0,1)}\big[(1-c)s\mathbf{1}(s \le c)\big] + \mathbf{E}_{c \sim U(0,1)}\big[c(1-s)\mathbf{1}(s > c)\big]\Big] \\
&\qquad\qquad\qquad\qquad\qquad\qquad\text{(exchanging expectations)} \\
&\quad= 2\mathbf{E}_s\Big[s\int_s^1 (1-c)\,dc + (1-s)\int_0^s c\,dc\Big] \\
&\quad= \mathbf{E}_s\big[s(1-s)^2 + (1-s)s^2\big] \\
&\quad= \mathbf{E}_s\big[\mathbf{P}(y=1|s)(1-s)^2 + \big(1 - \mathbf{P}(y=1|s)\big)s^2\big] \qquad \text{(since } \widehat{\eta} \text{ is calibrated)} \\
&\quad= \mathbf{E}_x\big[\eta(x)(1-\widehat{\eta}(x))^2 + \big(1-\eta(x)\big)\widehat{\eta}(x)^2\big] \\
&\qquad\qquad\qquad\text{(follows from } \mathbf{P}(y=1|s) = \mathbf{E}_x\big[\eta(x) \;\big|\; \widehat{\eta}(x) = s\big]\text{)} \\
&\quad= \text{er}_D^{\text{sq}}[\widehat{\eta}].
\end{aligned}$$

□

## D Proof of Lemma 11

*Proof.* Expanding the left hand side, we have

$$\begin{aligned}
\text{regret}_D^{\text{sq}}[\widehat{\eta}] &= \text{er}_D^{\text{sq}}[\widehat{\eta}] - \text{er}_D^{\text{sq},*} = \text{er}_D^{\text{sq}}[\widehat{\eta}] - \text{er}_D^{\text{sq}}[\eta] \\
&= 2\mathbf{E}_{c\sim U(0,1)}\big[\text{er}_D^{\text{0-1},c}\big[\text{Thresh}_{D,\widehat{\eta},c}\circ\widehat{\eta}\big]\big] - 2\mathbf{E}_{c\sim U(0,1)}\big[\text{er}_D^{\text{0-1},c}\big[\text{Thresh}_{D,\eta,c}\circ\eta\big]\big] \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(from Theorem 10)} \\
&= 2\mathbf{E}_{c\sim U(0,1)}\big[\text{er}_D^{\text{0-1},c}\big[\text{Thresh}_{D,\widehat{\eta},c}\circ\widehat{\eta}\big]\big] - 2\mathbf{E}_{c\sim U(0,1)}\big[\text{er}_D^{\text{0-1},c}\big[\text{sign}\circ(\eta - c)\big]\big] \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{(from Lemma 21)} \\
&= 2\mathbf{E}_{c\sim U(0,1)}\big[\text{er}_D^{\text{0-1},c}\big[\text{Thresh}_{D,\widehat{\eta},c}\circ\widehat{\eta}\big] - \text{er}_D^{\text{0-1},c,*}\big] \\
&\leq \sqrt{8p(1-p)\,\text{regret}_D^{\text{rank}}[\widehat{\eta}]} \quad \text{(from Theorem 4).}
\end{aligned}$$

□

## E Proof of Lemma 13

We will find it useful to introduce a few notations. For a given ranking model $f : X \to [a,b]$ and distribution $D$ over $X \times \{\pm 1\}$, define $\bar{\mu}_f(t) = \mathbf{P}(f(x) \leq t)$ and $\bar{\eta}_f(t) = \mathbf{P}(y = 1, f(x) \leq t)$ for all $t \in [a,b]$; as before, $p = \mathbf{P}(y = 1)$.

We first state a result of [27, 28] that characterizes the minimizer of (OP3).

**Theorem 22** ( [27, 28])**.** *Let $f : X \to [a,b]$ (where $a,b \in \mathbb{R}$, $a < b$) be any bounded-range ranking model and $D$ be any probability distribution over $X \times \{\pm 1\}$ such that $(D,f)$ satisfies Assumption A. Moreover assume that $\mu_f$ (see Assumption A), if mixed, does not have a point mass at the end-points $a,b$, and that the function $\eta_f : [a,b] \to [0,1]$ defined as $\eta_f(t) = \mathbf{P}(y = 1 \mid f(x) = t)$ is square-integrable w.r.t. the density of the continuous part of $\mu_f$. Then the minimizer $\text{Cal}_{D,f} : [a,b] \to [0,1]$ of (OP3) exists, and $\text{Cal}_{D,f}(\tau)$ for any $\tau \in (a,b)$ is given by the right-continuous slope of the largest convex minorant[5] of following graph at $t = \tau$:*

$$G[f] = \big\{\big(\bar{\mu}_f(t),\ \bar{\eta}_f(t)\big)\ :\ t \in [a,b]\big\}. \tag{5}$$

*Moreover, $G[\text{Cal}_{D,f} \circ f]$ is piece-wise linear on all portions where it disagrees with $G[f]$; in particular, there exists a collection of disjoint open intervals $\{(a_\alpha, b_\alpha) \mid \alpha \in \Lambda\}$ in $[a,b]$, where $\Lambda$ is some index set, such that $\text{Cal}_{D,f}$ evaluates to a constant on each such interval (with the constant being distinct for each interval) and $\text{Cal}_{D,f}$ is equal to $\eta_f$ everywhere else in $[a,b]$:*

$$\text{Cal}_{D,f}(t) = \begin{cases} \nu_\alpha & \text{if } t \in (a_\alpha, b_\alpha), \text{ for some } \alpha \in \Lambda \\ \eta_f(t) & \text{otherwise} \end{cases},$$

*where*

$$\nu_\alpha = \frac{\bar{\eta}_f(b_\alpha) - \bar{\eta}_f(a_\alpha)}{\bar{\mu}_f(b_\alpha) - \bar{\mu}_f(a_\alpha)}, \tag{6}$$

*with $\nu_\alpha \neq \nu_{\alpha'}$ for any $\alpha \neq \alpha'$, $\alpha, \alpha' \in \Lambda$.*

While the proof for the above result in [27, 28] assumes a continuous and strictly positive density $\mu_f$ over $[a,b]$, it can be extended to handle the slightly more general conditions considered here.

We are now ready to prove the two properties stated for $\text{Cal}_{D,f}$ in Lemma 13.

*Proof of Lemma 13.* We shall assume that the score distribution of $f$ over $[a,b]$ is continuous, and $\mu_f$ denotes the corresponding probability density function; a similar proof can be shown when the score distribution is discrete or is mixed and satisfies conditions stated in the Lemma. For simplicity of notation, let us denote $\text{Cal}_{D,f}$ as Cal.

*Proof of (1):* We need to show that for any $u \in \text{range}(\text{Cal} \circ f)$, $\mathbf{P}(y = 1 \mid \text{Cal}(f(x)) = u) = u$. There are three possible cases that we could consider: (i) $u = \nu_\alpha$, for some unique $\alpha \in \Lambda$ (see

[5] A real-valued function $g_1$ is a minorant of another real-valued function $g_2$ defined over the same domain, if $g_1(z) \leq g_2(z),\ \forall z$; similarly, $g_1$ is a majorant of $g_2$, if $g_1(z) \geq g_2(z),\ \forall z$.

Eq. (6)), with $\text{Cal}(t) = u, \forall t \in (a_\alpha, b_\alpha)$, and $\text{Cal}(t) \neq u$, for all $t \notin (a_\alpha, b_\alpha)$; (ii) $u \neq \nu_\alpha$, for any $\alpha \in \Lambda$; (iii) $u = \nu_\alpha$ for some unique $\alpha \in \Lambda$, and there exists $t \notin \cup_{\alpha\in\Lambda}(a_\alpha, b_\alpha)$ with $\text{Cal}(t) = u$.

For any $u \in \text{range}(\text{Cal} \circ f)$ satisfying case (i), there exists $\alpha \in \Lambda$ s.t. $\nu_\alpha = u$. We have from Eq. (6),

$$\begin{aligned} u &= \frac{\bar{\eta}_f(b_\alpha) - \bar{\eta}_f(a_\alpha)}{\bar{\mu}_f(b_\alpha) - \bar{\mu}_f(a_\alpha)} \\ &= \frac{\int_{a_\alpha}^{b_\alpha} \eta_f(s)\mu_f(s)ds}{\int_{a_\alpha}^{b_\alpha} \mu_f(s)ds} \\ &= \mathbf{P}\big(y = 1 \,\big|\, f(x) \in (a_\alpha, b_\alpha)\big) \\ &= \mathbf{P}\big(y = 1 \,\big|\, \text{Cal}(f(x)) = u\big). \end{aligned}$$

The last step follows from the fact that for all $t \notin (a_\alpha, b_\alpha)$, $\text{Cal}(t) \neq u$.

For any $u \in \text{range}(\text{Cal} \circ f)$ satisfying case (ii), there exists no $\alpha \in \Lambda$ with $\nu_\alpha = u$; we thus have from Theorem 22 that $\eta_f(t) = u$ for all $t$ with $\text{Cal}(t) = u$. Then

$$\begin{aligned} \mathbf{P}\big(y = 1 \,\big|\, \text{Cal}(f(x)) = u\big) &= \frac{\int_{\{s\,:\,\text{Cal}(s)=u\}} \eta_f(s)\mu_f(s)ds}{\int_{\{s\,:\,\text{Cal}(s)=u\}} \mu_f(s)ds} \\ &= \frac{\int_{\{s\,:\,\text{Cal}(s)=u\}} u\mu_f(s)ds}{\int_{\{s\,:\,\text{Cal}(s)=u\}} \mu_f(s)ds} \\ &= u. \end{aligned}$$

For any $u \in \text{range}(\text{Cal} \circ f)$ satisfying case (iii), there exists a unique $\alpha \in \Lambda$ for which $\nu_\alpha = u$, with $\text{Cal}(t) = u, \forall t \in (a_\alpha, b_\alpha)$, and there also exists $t \notin \cup_{\alpha\in\Lambda}(a_\alpha, b_\alpha)$, for which $\text{Cal}(t) = \eta_f(t) = u$.

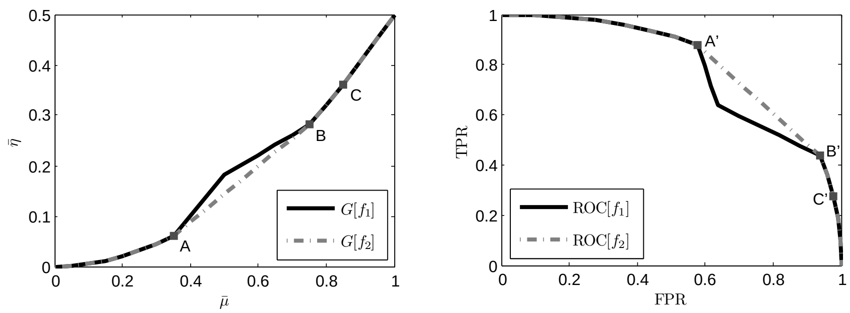
$$\begin{aligned} \mathbf{P}\big(y = 1 \,\big|\, \text{Cal}(f(x)) = u\big) &= \frac{\int_{\{s\,:\,\text{Cal}(s)=u\}} \eta_f(s)\mu_f(s)ds}{\int_{\{s\,:\,\text{Cal}(s)=u\}} \mu_f(s)ds} \\ &= \frac{\int_{a_\alpha}^{b_\alpha} \eta_f(s)\mu_f(s)ds \;+\; \int_{\{s\,:\,\text{Cal}(s)=\eta_f(s)=u\}} \eta_f(s)\mu_f(s)ds}{\int_{\{s\,:\,\text{Cal}(s)=u\}} \mu_f(s)ds} \\ &= \frac{u\int_{a_\alpha}^{b_\alpha} \mu_f(s)ds \;+\; u\int_{\{s\,:\,\text{Cal}(s)=\eta_f(s)=u\}} \mu_f(s)ds}{\int_{\{s\,:\,\text{Cal}(s)=u\}} \mu_f(s)ds} \\ &\qquad\qquad \text{(applying Eq. (6) to the first integral in the numerator)} \\ &= u. \end{aligned}$$

*Proof of (2):* Recall that for a ranking model $f$, $\text{er}_D^{\text{rank}}[f]$ is equivalent to one minus the area under the ROC curve[6] (AUC) of $f$. It is thus enough to show that the ROC curve of $\text{Cal} \circ f$ is a majorant for the ROC curve of $f$. The ROC curve for $f$ can be defined as

$$\begin{aligned} \text{ROC}[f] &= \Big\{\Big(\mathbf{P}(f(x) \leq t \mid y = -1),\ \mathbf{P}(f(x) > t \mid y = 1)\Big) \,:\, t \in [a, b]\Big\} \\ &= \Big\{\Big(\frac{1}{1-p}\int_a^t (1 - \eta_f(s))\mu_f(s)ds,\ \frac{1}{p}\int_t^b \eta_f(s)\mu_f(s)ds\Big) \,:\, t \in [a, b]\Big\}. \end{aligned} \tag{7}$$

As illustrated in Figure 4, each point in the graph $G[f]$ (defined in Eq. (5)) has a corresponding point in $\text{ROC}[f]$; similarly, each line segment in $G[f]$ corresponds to a line segment in $\text{ROC}[f]$. Moreover, for any two given ranking models $f_1$ and $f_2$, if a line segment in $G[f_1]$ is a minorant for a certain portion of $G[f_2]$, the corresponding line segment in $\text{ROC}[f_1]$ is a majorant for the corresponding portion of $\text{ROC}[f_2]$ (see segments AB and A'B' in Figure 4). Since, from Theorem 22, we have that $G[\text{Cal} \circ f]$ is a minorant for $G[f]$, and $G[\text{Cal} \circ f]$ is piece-wise linear on all portions where it disagrees with $G[f]$, it follows that $\text{ROC}[\text{Cal} \circ f]$ is a majorant for $\text{ROC}[f]$. □

[6]The ROC curve of a ranking model $f$ is the plot of the true positive rate (probability of classifying a random positive example as positive) against the false positive rate (probability of classifying a random negative example as positive) of a classifier of the form $\text{sign} \circ (f - t)$ for all thresholds $t \in [a, b]$.




(a) $G[f]$ (b) ROC$[f]$

Figure 4: Sample plots illustrating the relationship between the graph $G$ (plot of $\bar{\eta}_f(t)$ against $\bar{\mu}_f(t)$ for all $t \in [a, b]$; see Eq. (5)) and the ROC curve (plot of true positive rate $\text{TPR}_f(t) = \mathbf{P}(f(x) > t \mid y = 1)$ against false positive rate $\text{FPR}_f(t) = \mathbf{P}(f(x) \le t \mid y = -1)$ for all $t \in [a, b]$; see Eq. (7)). (a) Graph $G$ for ranking models $f_1$ and $f_2$: the graphs for $f_1$ and $f_2$ agree on all points except for the portion between points $A$ and $B$, where the line segment AB in $G[f_2]$ is a minorant for $G[f_1]$. (b) ROC curve for the ranking models $f_1$ and $f_2$: the points A, B and C in the graph $G$ for $f_1$ and $f_2$ correspond to points A', B' and C' respectively in the ROC curves for $f_1$ and $f_2$; the line segment AB in $G[f_2]$ corresponds to the line segment A'B' in ROC$[f_2]$, which is a majorant for the corresponding portion in ROC$[f_1]$. Moreover, while $G[f_2]$ is a convex minorant for $G[f_1]$, the corresponding ROC curve ROC$[f_2]$ is a concave majorant for ROC$[f_1]$.

## F Proof of Theorem 14

*Proof.* Using the fact that $\text{Cal}_{D,f} \circ f$ is calibrated (property 1 in Lemma 13), we have

$$\begin{aligned} \text{regret}^{\text{sq}}_D[\text{Cal} \circ f] &\le \sqrt{8p(1-p)\,\text{regret}^{\text{rank}}_D[\text{Cal}_{D,f} \circ f]} \quad \text{(from Lemma 11)} \\ &\le \sqrt{8p(1-p)\,\text{regret}^{\text{rank}}_D[f]} \quad \text{(from property 2 in Lemma 13).} \end{aligned}$$

□

## G Proof of Theorem 16

*Proof.*

$$\begin{aligned} \text{regret}^{\text{sq}}_D[\widehat{\text{Cal}}_{S,f} \circ f] &= \text{er}^{\text{sq}}_D[\widehat{\text{Cal}}_{S,f} \circ f] - \text{er}^{\text{sq}}_D[\eta] \\ &= \text{er}^{\text{sq}}_D[\widehat{\text{Cal}}_{S,f} \circ f] - \text{er}^{\text{sq}}_D[\text{Cal}_{D,f} \circ f] + \text{er}^{\text{sq}}_D[\text{Cal}_{D,f} \circ f] - \text{er}^{\text{sq}}_D[\eta] \\ &= \Big(\text{er}^{\text{sq}}_D[\widehat{\text{Cal}}_{S,f} \circ f] - \text{er}^{\text{sq}}_D[\text{Cal}_{D,f} \circ f]\Big) + \text{regret}^{\text{sq}}_D[\text{Cal}_{D,f} \circ f] \qquad (8) \end{aligned}$$

Using Theorem 14, the second term in the above expression can be upper bounded in terms of the ranking regret of $f$. We now focus on upper bounding the first term. As in the proof of Theorem 6, consider the distribution $D_f$ induced by $f$ over $\mathbb{R} \times \{\pm 1\}$ and let $S_f$ be the set obtained by applying $f$ to each instance in $S$; clearly, $S_f$ is iid drawn from $D_f$. One can then view the optimization problem in OP4 as empirical risk minimization over $\mathcal{G}_{\text{inc}}$ w.r.t. the sample $S_f$. Using standard Rademacher averages based uniform convergence result for empirical risk minimization over a real-valued function class with the squared loss, we have that the following holds with probability at least $1 - \delta$ (over the draw of $S \sim D^n$):

$$\text{er}^{\text{sq}}_D[\widehat{\text{Cal}}_{S,f} \circ f] - \inf_{g \in \mathcal{G}_{\text{inc}}} \text{er}^{\text{sq}}_D[g \circ f] \;\le\; 4R_{S_f}(\mathcal{G}_{\text{inc}}) \;+\; 2\sqrt{\frac{2\ln\left(\frac{8}{\delta}\right)}{n}},$$

where $R_{S_f}(\mathcal{G}_{\text{inc}})$ is the empirical Rademacher average of $\mathcal{G}_{\text{inc}}$ w.r.t. $S_f$. Using Dudley's integral, and bounds on covering numbers of $\mathcal{G}_{\text{inc}}$, one can show $R_{S_f}(\mathcal{G}_{\text{inc}}) \le 24\sqrt{\frac{2\ln(n)}{n}}$ (see for example [21]);

we thus have with probability at least $1-\delta$ (over the draw of $S \sim D^n$),

$$\mathrm{er}_D^{\mathrm{sq}}[\widehat{\mathrm{Cal}}_{S,f} \circ f] - \inf_{g \in \mathcal{G}_{\mathrm{inc}}} \mathrm{er}_D^{\mathrm{sq}}[g \circ f] \;\leq\; 96\sqrt{\frac{2\ln(n)}{n}} + 2\sqrt{\frac{2\ln\left(\frac{8}{\delta}\right)}{n}}.$$

Plugging this into Eq. (8) (along with the upper bound on the second term) completes the proof. $\square$