What about stronger guarantees than marginal?

Let's focus on regression

$Y = [0,1]$, goal is

$$f^*(x) = \mathbb{E}[y \mid x]$$

think squared error $\mathbb{E}[(y - f(x))^2]$

What about thinking of f as estimating $y \mid x$ ... eg. if $f(x) = v$

$$\cancel{\mathbb{E}[f(y) = v \mid x : f(x) = v]}$$

$$\mathbb{E}[y \mid f(x) = v] = v \quad \forall v \, ?$$

f is correct on average | on its own pred.

~~Type~~ Measuring miscalibration:

$$ACE(f, D) = \sum_{v \in R(f)} \Pr[f(x) = v] \, | v - \mathbb{E}[y \mid f(x) = v] |$$

$$SCE(f, D) = \sum_{v \in R(f)} (\qquad)^2$$

$$MCE(f, D) = \max_{v}$$

These are all Related $|R(f)| = m$

$$K_2(f) \le K_1(f) \le \sqrt{K_2(f)}$$

$$K_\infty(f) \le K_1(f) \le m \cdot K_\infty(f)$$

Squared error is almost never 0, but $SCE(f^*) = 0$, if f^* mins ^{2}error

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How do we "fix" Miscalibration?

A: for any v s.t. $\mathbb{E}[y \mid f(x)=v] \ne v$

Set ~~$\mathbb{E}[f(x)=v]$~~

$\forall x_{old}$ $\quad f_{new}(x_{old}) = \mathbb{E}[y \mid f_{old}(x) = v]$

Calibrate$(f, \alpha$

Let $f_0 = f$, $t=0$

While ($K_2(f_t$

Let

$v_t \in$ ar

$v'_t = \mathbb{E}$

Let $f_{t+1} =$ h

Output f_t

Claim: each

Lemma

Let $v^* = \mathbb{E}[y$ $\quad y \sim \mathcal{D}_y$

$\mathbb{E}[($

Pf $= \mathbb{E}[$

$= \mathbb{E}[$

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$\mathbb{E}$

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Calibrate(f, α, D)

Let $f_0 = f$, $t=0$

While ($K_2(f_t, D) > \alpha$) do

Let $v_t \in \arg\max_v \Pr[f_t(x) = v] \, (v - E[y \mid f_t(x) = v])^2$

$v_t' = E[y \mid f_t(x) = v_t]$

Let $f_{t+1} = h(x; f_t, v_t \Rightarrow v_t')$, $t = t+1$

Output f_t

$$h(x, f, v \Rightarrow v') = \begin{cases} f(x) & \text{if } f(x) \neq v \\ v' & \text{if } f(x) = v \end{cases}$$

Claim: each iteration improves $K_2(f_t, D)$

Lemma

Let $v^* = \mathop{E}_{y \sim D_y}[y]$, $\hat{v} = v^* + \Delta$, $\Delta \neq 0$. Then

$$E[(\hat{v} - y)^2 - (v^* - y)^2] = \Delta^2$$

Pf

$$= E[\hat{v}^2 - 2\hat{v}y - \cancel{y^2} - v^{*2} + 2yv^* \cancel{+y^2}]$$

$$= E[\hat{v}^2 - 2\hat{v}y - v^{*2} + 2v^*y]$$

$$E[(v^* + \Delta)^2 - 2(v^* + \Delta)y - v^{*2} + 2v^*y]$$

$$E[\underline{v^{*2}} + 2\Delta v^* + \Delta^2 - 2v^*y - 2\Delta y - \underline{v^{*2}} + 2v^*y]$$

$$E[2\Delta v^* + \Delta^2 - \underline{2v^*y} - 2\Delta y + \underline{2v^*y}]$$

$$= E[2\Delta v^* + \Delta^2 - 2\Delta y]$$

$$= 2\Delta v^* + \Delta^2 - 2v^*\Delta$$

$$= \Delta^2$$

So, patching is good!
Each iter must find a v s.t.

$$\Delta_t = \Pr[f_t(x) = v_t]\left(v_t - \mathbb{E}[y \mid f(x) = v_t]\right)^2 \geq \frac{\alpha}{m}$$

since $K_2 \geq \alpha$ $\exists$ one of m values

$$(v_t - v_t')^2 = \frac{\Delta_t}{\Pr[f(x_t) = v_t]}$$

$L_2(f_{t+1}) \geq L_2(f_t)$

$$= \Pr[f_t(x) = v_t]\left(K_2(f_{t+1} \mid v_t) - K_2(f_t \mid v_t)\right)$$
$$+ \Pr[f_t(x) \neq v_t](\text{equal error})$$
$$= \Pr[f_t(x) = v_t](v_t' - v_t)^2 = \Delta_t \quad (\text{Lemma})$$
$$\geq \frac{\alpha}{m}$$

So error drops by $\geq \frac{\alpha}{m}$, is ≤ 1 and ≥ 0, so after $\frac{m}{\alpha}$ rounds will halt w/ error $< \alpha$

Simpler alg works too: Patch everywhere @ once. Then $K_2(f') = 0$, $L_2(f') = L_2(f) - K_2(f)$.

You might also wan
q:

Def'l Average quant
is

$$Q_1(f) = \sum_{v \in R(f)} \Pr[$$

& squared is

$$Q_2(f) = \sum \Pr[$$

& max is

$$Q_\infty(f) = \max_{v \in R(f)}$$

[And, just like

To fix QCE, y
$\forall v \in R(f)$

Output

You might also want <u>quantile</u> calibration for a quantile q:

<u>Def</u> Average quantile calibration error of f for q is

$$Q_1(f) = \sum_{v \in R(f)} \Pr[f(x)=v] \, \left| q - \Pr[y \le v \mid f(x)=v] \right|$$

& squared is

$$Q_2(f) = \sum \Pr[f(x)=v] \left(q - \Pr[y \le v \mid f(x)=v]\right)^2$$

& max is

$$Q_\infty(f) = \max_{v \in R(f)} \Pr[f(x)=v] \left| q - \Pr[y \le v \mid f(x)=v] \right|$$

[And, just like K_1, K_2, K_∞, $\quad Q_2(f) \le Q_1(f) \le \sqrt{Q_2(f)}$

$Q_\infty(f) \le Q_1(f) \le m \, Q_\infty(f)$

To fix QCE, you can patch everywhere @ once

$\forall v \in R(f)$ let

$$c(v) = \underset{v'}{\operatorname{argmin}} \left| q - \Pr[y \le v' \mid f(x)=v] \right|$$

amongst pts where $f(x)=v$ find the q-quantile value v'

Output $\hat{f}(x) = c(f(x))$

As promised, we'll think about these in online instead of just distributional, batch settings.

Consider a transcript Π w predictions $p_t \in \{0, \frac{1}{m}, .. 1\}$

Define Avg ^{2} Mean (+ Q) Calibration error

$$n(\Pi, p) = \sum_{t=1}^{T} \mathbb{1}(p_t = p)$$

$$K_2(\Pi) = \sum_{p \in [\frac{1}{m}]} \frac{n(\Pi, p)}{T} \left(\frac{\sum \mathbb{1}(p_t = p)(y_t - p_t)}{n(\Pi, p)} \right)^2 = \frac{1}{T} \sum_{p \in [\frac{1}{m}]} \left(\frac{\sum_{t=1}^{T} \mathbb{1}(p_t = p)(y_t - p_t)}{\sqrt{n(\Pi, p)}} \right)^2$$

$\bar{K}_2(\Pi) = T K_2(\Pi)$ (unnormalized)

Calculate your miscalibration so far till rd s:

$$V_s^p(\Pi) = \sum_{t=1}^{s} \frac{\mathbb{1}(p_t = p)(y_t - p_t)}{\sqrt{n(\Pi^{\leq s}, p)}}$$

Then [Lemma]

$$\Delta_{s+1}(p_{s+1}, y_{s+1}) = \bar{K}_2(\Pi^{\leq s+1}) - \bar{K}_2(\Pi^{\leq s})$$

$$\leq \frac{2 V_s^{p_{s+1}}}{\sqrt{n(\Pi^{\leq s}, p_{s+1})}} (y_s - p_{s+1}) + \frac{1}{n(\Pi^{\leq s}, p_{s+1})}$$

$\cancel{\text{Also}}$ $($ p $V_s^p(\Pi) \leq \sqrt{n(\Pi^{\leq s}, p)}$

Since

$$\sum_{t=1}^{s} \mathbb{1}(p_t = p) = n(\Pi^{\leq s}, p)$$

The only terms in $\bar{K}_2$ that change are those w $p = p_{s+1}$

$$\Delta = \left(\frac{\sum^{s+1} \mathbb{1}(p_t = p_{s+1})(y_t - p_t)}{\sqrt{n(\Pi^{\leq s+1}, p_{s+1})}} \right)^2 - \left(\frac{\sum^{s} \mathbb{1}(p_t = p_{s+1})(y_t - p_t)}{\sqrt{n(\Pi^{\leq s}, p_{s+1})}} \right)^2$$

$$\left(\frac{\quad}{\sqrt{n(\Pi^{\leq s}, p_{s+1})}} \right)^2$$

se in online

ngs.

tions $p_t \in \{0, \frac{1}{m}, \dots, 1\}$

or

$$\frac{1}{T} \sum_{p \in [\frac{1}{m}]} \left(\frac{\sum_{t=1}^{T} \mathbb{1}(p_t = p)(y_t - p_t)}{\sqrt{n(\Pi, p)}} \right)^2$$

:

$\phi(p \qquad V_s^{p}(\Pi) \le \sqrt{n(\Pi^{\le s}, p)}$

since

$\mathbb{1}(p_t = p) =$

$n(\Pi^{\le s}, p)$

those w $p = p_{s+1}$

$$)(y_t - p_t) \Big)^2 \qquad , p_{s+1})$$

$$= \left(V_s^{p_{s+1}}(\Pi^{\le s}) + \frac{y_{s+1} - p_{s+1}}{\sqrt{n(\Pi^{\le s}, p_{s+1})}} \right)^2 - V_s^{p_{s+1}}(\Pi^{\le s})^2$$

$$= 2 V_s^{p_{s+1}}(\Pi^{\le s}) \left(\qquad \right) + \frac{(y_{s+1} - p_{s+1})^2}{n(\Pi^{\le s}, p_{s+1})}$$

$$\le \frac{2 V_s^{p_{s+1}} (y_{s+1} - p_{s+1})}{\sqrt{n(\Pi^{\le s}, p_{s+1})}} + \frac{1}{n(\Pi^{\le s}, p_{s+1})}$$

So if $\forall \Pi$, $\exists$ a dist over predictions p_{s+1} that makes this small $\forall$ y_{s+1},

anway playing that will have small CE online.

Name this term $\Delta'_{s+1}(p_{s+1}, y_{s+1})$. Want $E[\Delta'_{s+1}(\,)]$ small.

Sample: