On the Calibration of Multiclass Classification with Rejection

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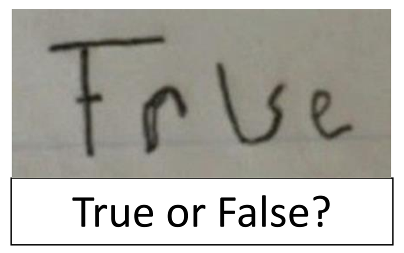
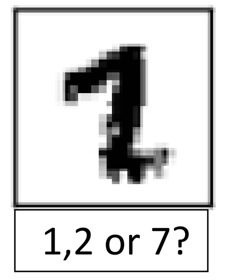
Introduction: Learning with rejection



Source: https://me.me/i/the-right-way-to-answer-true-and-false-questions-18781463



Source: MNIST dataset Lecun (1998)

Saying **"I don't know"** can **prevent misclassification**.

Related work: Most theoretical works in this problem focused on binary case.

Approach	Binary	Multiclass
Confidence-base	Bartlett+ (2008); Yuan+ (2010)	Ramaswamy+ (2018)
Classifier-rejector	Cortes+ (2015, 2016)	X

Contributions:

- **Calibration condition for surrogate losses in the classifier-rejector approach, which suggests the difficulty especially in the multiclass case**
- **Excess risk bounds and estimation error bounds to guarantee the one-vs-all (OVA) and cross-entropy (CE) losses in the confidence-based approach**

Multiclass classification with rejection

Chow (1970); Ramaswamy+ (2018)

Given: Labeled data: $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} p(\boldsymbol{x}, y)$

Rejection cost: $c \in (0, 0.5)$

$\boldsymbol{x} \in \mathcal{X} \subseteq \mathbb{R}^d$, $y \in \mathcal{Y} = \{1, \ldots, K\}$, $g_i(\boldsymbol{x}) \colon \mathcal{X} \to \mathbb{R}$

Find: Classifier: $f(\boldsymbol{x}) = \underset{y \in \mathcal{Y}}{\operatorname{argmax}}\, g_y(\boldsymbol{x})$

Rejector: $r \colon \mathcal{X} \to \mathbb{R}$

$$\text{decision}(\boldsymbol{x}) = \begin{cases} f(\boldsymbol{x}), r(\boldsymbol{x}) > 0 \\ \text{reject}, r(\boldsymbol{x}) \le 0 \end{cases}$$

Goal: Minimize $R_{\text{0-1-}c}(r, f) = \underset{p(\boldsymbol{x}, y)}{\mathbb{E}}[\mathcal{L}_{\text{0-1-}c}(r, f; \boldsymbol{x}, y)]$

where $\mathcal{L}_{\text{0-1-}c}(r, f; \boldsymbol{x}, y) = \underbrace{\mathbb{1}_{[f(\boldsymbol{x}) \neq y]} \mathbb{1}_{[r(\boldsymbol{x}) > 0]}}_{\text{misclassification loss}} + \underbrace{c \mathbb{1}_{[r(\boldsymbol{x}) \le 0]}}_{\text{rejection loss}}$

$\mathcal{L}_{\text{0-1-}c}(r, f; \boldsymbol{x}, y)$ **is difficult to directly optimize.**

Yuan+ (2010); Cortes+ (2015, 2016); Ramaswamy+ (2018)

A computationally-efficient and theoretically justified surrogate loss is needed.

Calibration

Calibration ensures that minimizing a surrogate loss will lead to an optimal solution.

Optimal solution of classification with rejection: Chow (1970)

$$f^*(\boldsymbol{x}) = \underset{y \in \mathcal{Y}}{\arg\max}\, \eta_y(\boldsymbol{x}) \qquad \eta_y(\boldsymbol{x}) = p(y|\boldsymbol{x})$$

$$r^*(\boldsymbol{x}) = \max_{y \in \mathcal{Y}} \eta_y(\boldsymbol{x}) - (1 - c)$$

- (r, f) is **calibrated** if $R_{\text{0-1-}c}(r, f) = R_{\text{0-1-}c}(r^*, f^*)$.
- f is **classification-calibrated** if $f(\boldsymbol{x}) = f^*(\boldsymbol{x})$.
- r is **rejection-calibrated** if $\operatorname{sign}[r(\boldsymbol{x})] = \operatorname{sign}[r^*(\boldsymbol{x})]$.

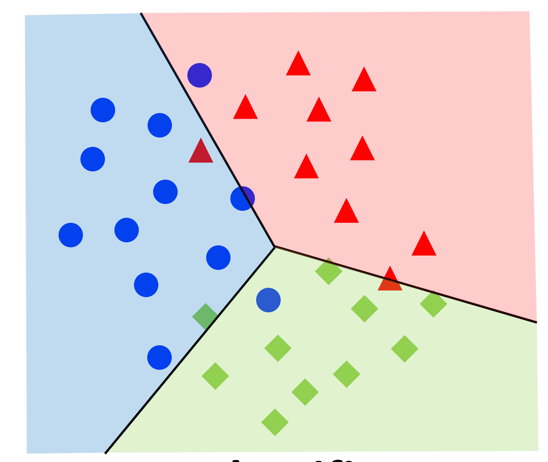
If (r, f) is calibrated, r must be rejection-calibrated.

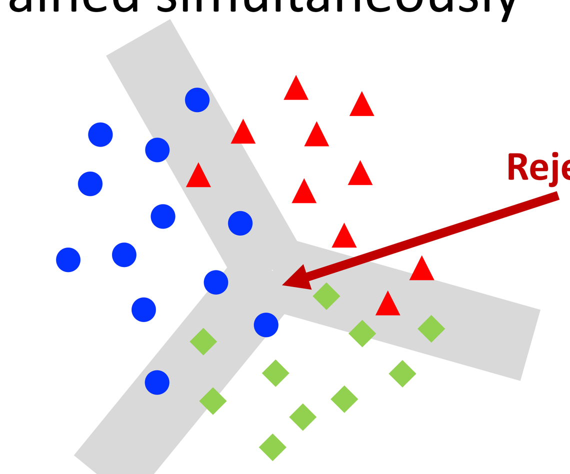
A minimizer of a surrogate loss should give a calibrated (r, f).

Classifier-rejector approach

Cortes+ (2015, 2016)

Classifier and **rejector** are trained simultaneously


Classifier



Rejector

Cortes+ (2015, 2016) proposed this approach in binary case:

- State-of-the-art method in binary case.
- Rejector is flexible, which is desirable when classifier model is misspecified.

$(r^\dagger_{\boldsymbol{\eta}}, f^\dagger_{\boldsymbol{\eta}}) = \underset{r \in \mathbb{R},\, \boldsymbol{g} \in \mathbb{R}^K}{\arg\min}\, W(r, f; \boldsymbol{\eta})$ $\quad \boldsymbol{\eta}(\boldsymbol{x}) = [\eta_1(\boldsymbol{x}), \ldots, \eta_K(\boldsymbol{x})]^\top$ $\quad W(r(\boldsymbol{x}), f(\boldsymbol{x}); \boldsymbol{\eta}(\boldsymbol{x})) = \sum_{y \in \mathcal{Y}} \eta_y(\boldsymbol{x}) \mathcal{L}(r, f; \boldsymbol{x}, y)$

Corollary 5: (Necessary condition for rejection calibration)

For $\mathcal{L}(r, f; \boldsymbol{x}, y)$ that is convex with respect to r and $\left.\frac{\partial^2 W(r, f^\dagger_{\boldsymbol{\eta}}; \boldsymbol{\eta})}{\partial r^2}\right|_{r=0} > 0$ **$r^\dagger$ is rejection-calibrated only if both conditions hold:**

Condition (1)

$$\underbrace{\sup_{\boldsymbol{\eta}:\, \max_y \eta_y = 1 - c} \left.\frac{\partial W(r, f^\dagger_{\boldsymbol{\eta}}; \boldsymbol{\eta})}{\partial r}\right|_{r=0} = 0}_{\text{Condition for false reject rate to be zero}}$$

Condition (2)

$$\underbrace{\inf_{\boldsymbol{\eta}:\, \max_y \eta_y = 1 - c} \left.\frac{\partial W(r, f^\dagger_{\boldsymbol{\eta}}; \boldsymbol{\eta})}{\partial r}\right|_{r=0} = 0}_{\text{Condition for false accept rate to be zero}}$$

A necessary and sufficient condition is also provided in our paper (Theorem 4)

Supremum and infimum values coincide under the same constraint.

When $\max_y \eta_y = 1 - c$

- Binary case: $\boldsymbol{\eta}$ can only be either $[1 - c, c]^\top$ or $[c, 1 - c]^\top$.
- Multiclass case: $\boldsymbol{\eta}$ **has infinitely many candidates!**

Case study:

$\alpha \in \mathbb{R}$ $\beta \in \mathbb{R}$ Hyperparameters

$\phi \colon \mathbb{R} \to \mathbb{R}$ $\psi \colon \mathbb{R} \to \mathbb{R}$ Convex margin losses

- **Multiplicative pairwise comparison (MPC) loss:**

$$\mathcal{L}_{\text{MPC}}(r, f; \boldsymbol{x}, y) = \sum_{y' \neq y} \phi\Big(\alpha\big(g_y(\boldsymbol{x}) - g_{y'}(\boldsymbol{x})\big)\Big)\psi(-\alpha r(\boldsymbol{x})) + c\psi(\beta r(\boldsymbol{x}))$$

- **Additive pairwise comparison (APC) loss:**

$$\mathcal{L}_{\text{APC}}(r, f; \boldsymbol{x}, y) = \sum_{y' \neq y} \phi\Big(\alpha\big(g_y(\boldsymbol{x}) - g_{y'}(\boldsymbol{x}) - r(\boldsymbol{x})\big)\Big) + c\psi(\beta r(\boldsymbol{x}))$$

Consider $\phi(z) = \psi(z) = \exp(-z)$

Condition (1) gives $\frac{\beta}{\alpha} = (K - 2) + 2\sqrt{(K - 1)\frac{1 - c}{c}}$

Condition (2) gives $\frac{\beta}{\alpha} = 2\sqrt{\frac{1 - c}{c}}$

Equivalent to the result by Cortes+ (2016) when considering a binary case $(K = 2)$.

In multiclass case, (α, β) **satisfying both conditions does not exist.**

Similar results also hold when using the logistic loss $\phi(z) = \psi(z) = \log(1 + \exp(-z))$.

References

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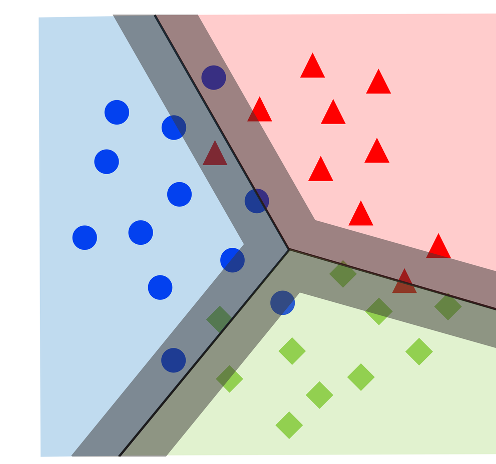
Confidence-based approach

Bartlett+ (2008); Yuan+ (2010); Ramaswamy+ (2018)

Rejector depends solely on **classifier's** confidence



- **Cross-entropy (CE) loss:**

$$\mathcal{L}_{\text{CE}}(f; \boldsymbol{x}, y) = -g_y(\boldsymbol{x}) + \log \sum_{y' \in \mathcal{Y}} \exp\left(g_{y'}(\boldsymbol{x})\right)$$

- **One-versus-all (OVA) loss:**

$$\mathcal{L}_{\text{OVA}}(f; \boldsymbol{x}, y) = \phi\big(g_y(\boldsymbol{x})\big) + \sum_{y' \neq y} \phi\big(-g_{y'}(\boldsymbol{x})\big)$$

- **Rejector:** $\quad \boldsymbol{g}(\boldsymbol{x}) = [g_1(\boldsymbol{x}), \ldots, g_K(\boldsymbol{x})]^\top$

$$r_f(\boldsymbol{x}) = \max_{y \in \mathcal{Y}} \Psi^{-1}(\boldsymbol{g}(\boldsymbol{x})) - (1 - c)$$

$\Psi^{-1} \colon \mathbb{R}^K \to [0, 1]^K$ Inverse link function

$\Psi^{-1}_{y,\,\text{OVA}}(\boldsymbol{g}) = \frac{\phi'(-g_y)}{\phi'(-g_y) + \phi'(g_y)}$ See our paper for conditions on ϕ.

$\Psi^{-1}_{y,\,\text{CE}}(\boldsymbol{g}) = \frac{\exp(g_y)}{\sum_{y' \in \mathcal{Y}} \exp(g_{y'})}$ Softmax function

Minimizers of **OVA** and **CE** losses also minimize the **0-1-c** loss

-> this can be justified by **excess risk bounds!**

Excess risk:

$$\Delta R_{\text{0-1-}c}(r_f, f) = R_{\text{0-1-}c}(r_f, f) - \inf_{f'\text{:measurable}} R_{\text{0-1-}c}(r_f, f)$$

$$\Delta R_\ell(f) = R_\ell(f) - \inf_{f'\text{:measurable}} R_\ell(f')$$

Excess risk bound of OVA loss:

$$(2C)^{-s} \Delta R_{\text{0-1-}c}(r_f, f)^s \le \Delta R_{\text{OVA}}(f)$$

Loss Name	$\phi(z)$	C	s
Logistic	$\log(1 + \exp(-z))$	$\frac{1}{2}$	2
Exponential	$\exp(-z)$	$\frac{1}{\sqrt{2}}$	2
Squared	$(1 - z)^2$	$\frac{1}{2}$	2
Squared Hinge	$(1 - z)_+^2$	$\frac{1}{2}$	2

Extension of the result by **Yuan+ (2010)** to the multiclass case.

Excess risk bound of CE loss:

$$\frac{1}{2} \Delta R_{\text{0-1-}c}(r_f, f)^2 \le \Delta R_{\text{CE}}(f)$$

Proof by case analysis: rewrites excess risk using KL-divergence and uses the Pinsker's inequality.

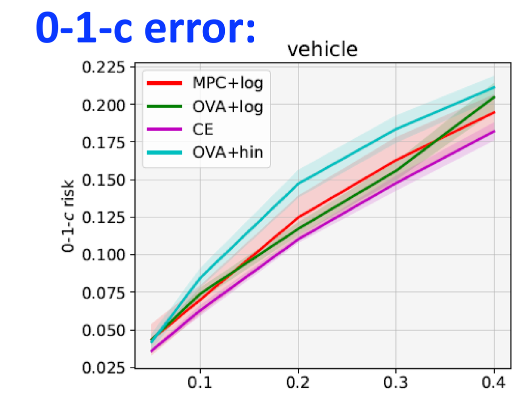
See our paper for more results, e.g., estimation error bound using Rademacher complexity.

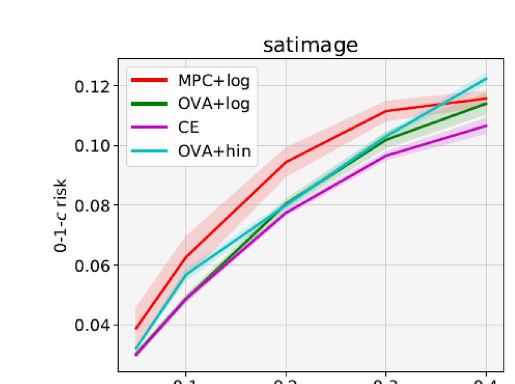
Experiments

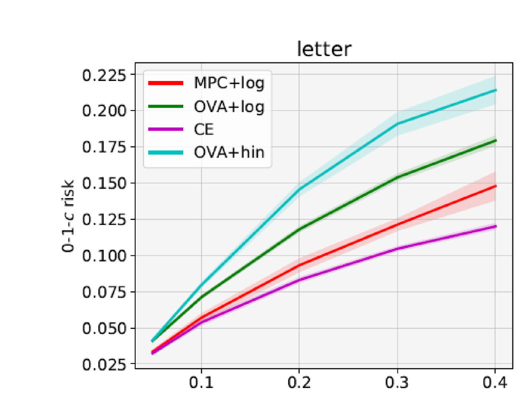
Classifier-rejector: MPC+log (MPC with logistic loss), APC+log (APC with logistic loss)

Confidence-based: OVA+hin by Ramaswamy+ (2018), OVA+log (OVA with logistic loss), CE

0-1-c error:







Accuracy of non-rejected data: "- (-)" indicates all data were rejected.

dataset	c	APC+log	MPC+log	OVA+log	CE
vehicle	0.05	- (-)	96.6 (2.3)	100 (0.0)	**100 (0.0)**
	0.2	98.4 (1.9)	92.4 (3.0)	97.9 (0.7)	**97.4 (0.1)**
	0.4	**89.1 (2.9)**	85.3 (4.2)	90.2 (1.6)	**91.7 (0.9)**
satimage	0.05	**99.1 (0.2)**	97.2 (1.4)	**98.7 (0.1)**	**98.3 (0.1)**
	0.2	95.0 (1.0)	92.6 (1.2)	96.2 (0.2)	**95.7 (0.1)**
	0.4	91.5 (0.7)	89.0 (1.1)	92.2 (0.3)	**91.8 (0.2)**
yeast	0.05	- (-)	- (-)	- (-)	- (-)
	0.2	- (-)	- (-)	- (-)	**80.6 (6.2)**
	0.4	- (-)	- (-)	75.0 (3.9)	**76.6 (1.7)**

dataset	c	APC+log	MPC+log	OVA+log	CE
covtype	0.05	**79.5 (2.1)**	79.8 (1.7)	**82.1 (2.7)**	**82.0 (3.2)**
	0.2	74.0 (1.8)	73.8 (1.0)	74.9 (1.4)	**77.1 (0.3)**
	0.4	**69.8 (1.3)**	64.9 (3.4)	**68.7 (1.1)**	**69.4 (1.8)**
letter	0.05	**99.8 (0.1)**	98.6 (0.2)	**99.6 (0.2)**	**99 8 (0.0)**
	0.2	97.9 (0.3)	96.9 (0.5)	**98.3 (0.2)**	**98.4 (0.1)**
	0.4	**95.2 (0.5)**	94.6 (3.8)	94.6 (0.2)	**94.9 (0.3)**