EnsLoss: Stochastic Calibrated Loss Ensembles for Preventing Overfitting in Classification

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Background

The objective of binary classification is to categorize each instance into one of two classes.

- **Data**: $\mathbf{X} \in \mathbb{R}^d \to Y \in \{-1, +1\}$
- **Classifier**: $f(\mathbf{X}) : \mathbb{R}^d \to \mathbb{R}$
- **Predicted label**: $\widehat{Y} = \operatorname{sgn}(f(\mathbf{X}))$
- **Evaluation** via Misclassification error **(risk)**:

$$R(f) = 1 - \mathrm{Acc}(f) = \mathbb{E}(\mathbf{1}(Yf(\mathbf{X}) \leq 0)),$$

where $\mathbf{1}(\cdot)$ is an indicator function.

Aim. To obtain *the Bayes classifier* or the best classifier:

$$f^* := \arg\min R(f)$$

Background

Due to the **discontinuity** of the indicator function:

$$R(f) = 1 - \mathrm{Acc}(f) = \mathbb{E}\big(\boxed{\mathbf{1}(Yf(\mathbf{X}) \leq 0)}\big),$$

the zero-one loss is usually replaced by a ***convex*** and ***classification-calibrated*** loss ϕ to facilitate the empirical computation (Lin, 2004; Zhang, 2004; Bartlett et al., 2006):

$$R_\phi(f) = \mathbb{E}(\phi(Yf(\mathbf{X})))$$

For example, the hinge loss for SVM, exponential loss for AdaBoost, and logistic loss for logistic regression all follow this framework.

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(If we optimize with respect to ϕ, will the resulting solution still be the function f^* that we need?)

That's why we need the loss ϕ to be **calibrated**?

Background

Definition 1 (Bartlett et al. (2006)). A loss function $\phi(\cdot)$ is classification-calibrated, if for every sequence of measurable function f_n and every probability distribution on $\mathcal{X} \times \{\pm 1\}$,

$$R_\phi(f_n) \to \inf_f R_\phi(f) \text{ implies that } R(f_n) \to \inf_f R(f).$$

A **calibrated** loss function ϕ guarantees that any sequence f_n that optimizes R_ϕ will eventually also optimize R, thereby ensuring **consistency** in maximizing classification accuracy.

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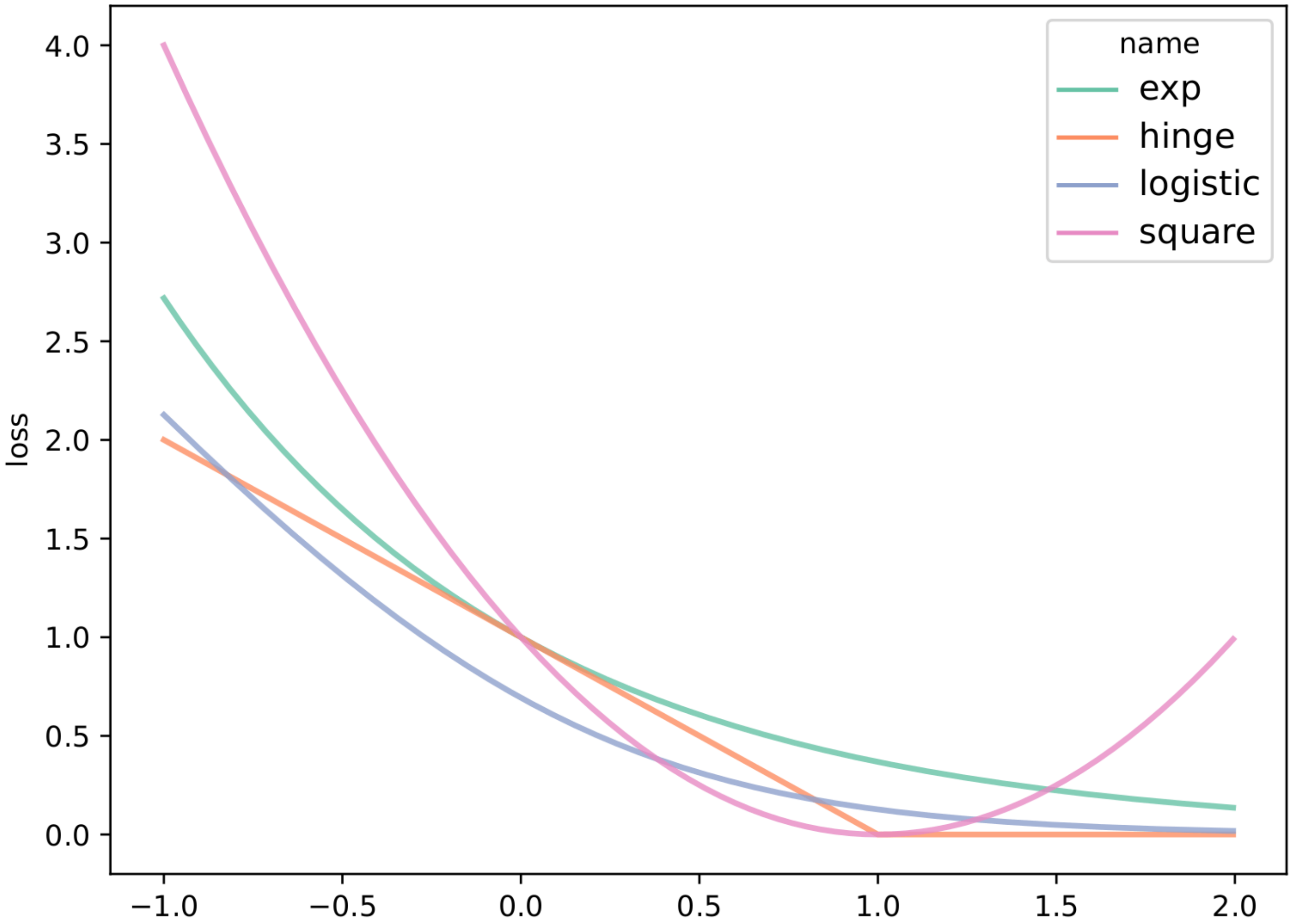
A series of studies (Lin, 2004; Zhang, 2004; Bartlett et al., 2006) culminates in the following theorem for **iff conditions** of calibration:

Theorem 1 (Bartlett et al. (2006)) Let ϕ be convex. Then ϕ is classification-calibrated iff it is differentiable at 0 and $\phi'(0) < 0$.

Classification ERM framework

(i) Select a **convex** and **calibrated** (CC) loss function ϕ



Classification ERM framework

(i) Select a **convex** and **calibrated** (CC) loss function ϕ

(ii) Directly minimizes the **ERM** of R_ϕ to obtain f_n

$$\hat{f}_n = \operatorname*{arg\,min}_{f \in \mathcal{F}} \ \widehat{R}_\phi(f), \quad \widehat{R}_\phi(f) := \frac{1}{n} \sum_{i=1}^{n} \phi\big(y_i f(\mathbf{x}_i)\big).$$

(SGD is widely adopted for its scalability and generalization when dealing with large-scale datasets and DL models)

$$\begin{aligned} \theta^{(t+1)} &= \theta^{(t)} - \gamma \frac{1}{B} \sum_{i \in \mathcal{I}_B} \nabla_\theta \phi(y_i f_{\theta^{(t)}}(\mathbf{x}_i)) \\ &= \theta^{(t)} - \gamma \frac{1}{B} \sum_{i \in \mathcal{I}_B} \partial \phi(y_i f_{\theta^{(t)}}(\mathbf{x}_i)) \nabla_\theta f_{\theta^{(t)}}(\mathbf{x}_i), \end{aligned}$$

The **ERM** paradigm with **calibrated losses**, when combined with **ML/DL models** and optimized using **SGD**, has achieved tremendous success in numerous real-world applications.

EnsLoss: Calibrated Loss Ensembles

SGD + Fixed Loss

For each iteration:

- batch sampling from a training set;
- implement SGD on batch samples and *a fixed surrogate loss*.

SGD + Ensemble Loss (ENSLOSS; our)

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Inspired by **Dropout**

(model ensemble over one training process)

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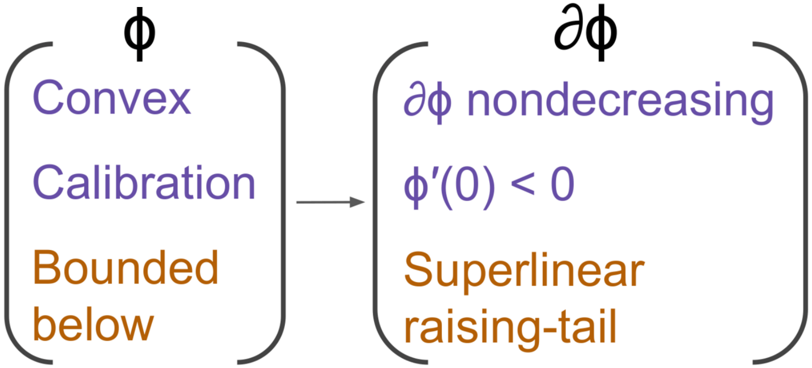

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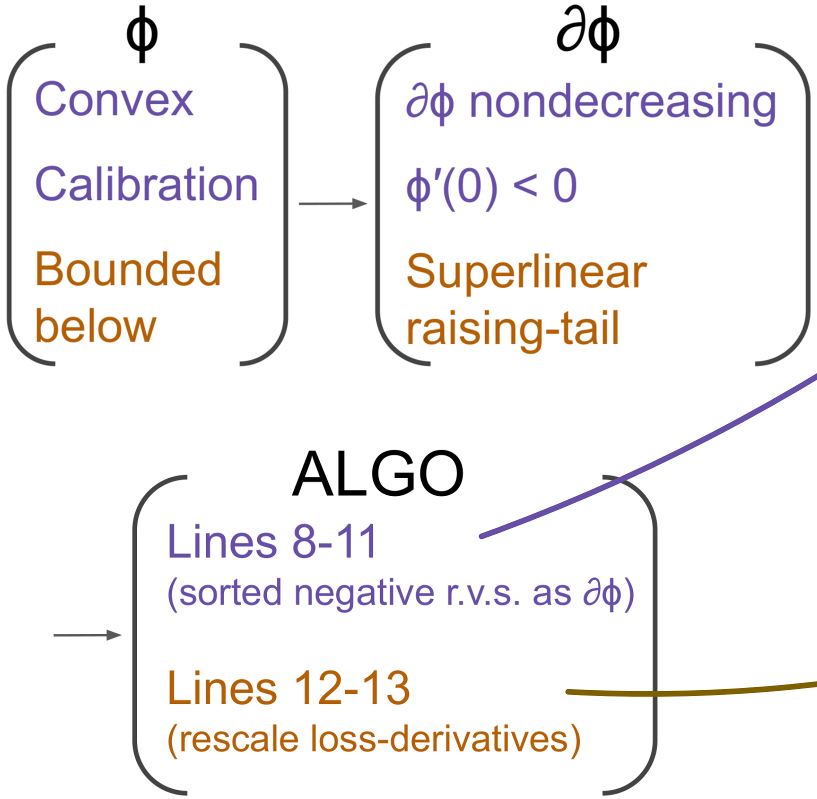
EnsLoss



Algorithm 1 (Minibatch) Calibrated ensemble SGD.

1: **Input:** a train set $\mathcal{D} = (x_i, y_i)_{i=1}^n$, a minibatch size B;
2: Initialize $\boldsymbol{\theta}$.
3: **for** number of epoches **do**
4: `/* Minibatch sampling */`
5: Sample a minibatch from $\mathcal{D}$ *without* replacement: $\mathcal{B} = \{(\mathbf{x}_{i_1}, y_{i_1}), \cdots, (\mathbf{x}_{i_B}, y_{i_B})\}$.
6: Compute $\mathbf{z} = (z_1, \cdots, z_B)^\intercal$, where $z_b = y_{i_b} f_{\boldsymbol{\theta}}(\mathbf{x}_{i_b})$ for $b = 1, \cdots, B$.
7: `/* Generate random RC loss-derivs */`
8: `/* calibration and convexity */`
9: Generate $\mathbf{g} = (g_1, \cdots, g_B)^\intercal$, where $g_b \overset{iid}{\sim} -\xi$, where ξ is a *positive random variable* (accomplished through Algorithm 2)
10: Sort $\mathbf{z}$ and $\mathbf{g}$ decreasingly, that is

$$z_{\pi(1)} > \cdots > z_{\pi(B)}, \quad g_{\sigma(1)} > \cdots > g_{\sigma(B)};$$

11: (the derivative corresponding to z_b is $g_{\sigma(\pi^{-1}(b))}$).
12: `/* bounded below */`
13: For $b = 1, \cdots, B$,

$$g_{\sigma(\pi^{-1}(b))} \leftarrow g_{\sigma(\pi^{-1}(b))}/z_b, \quad \text{if } z_b > 1.$$

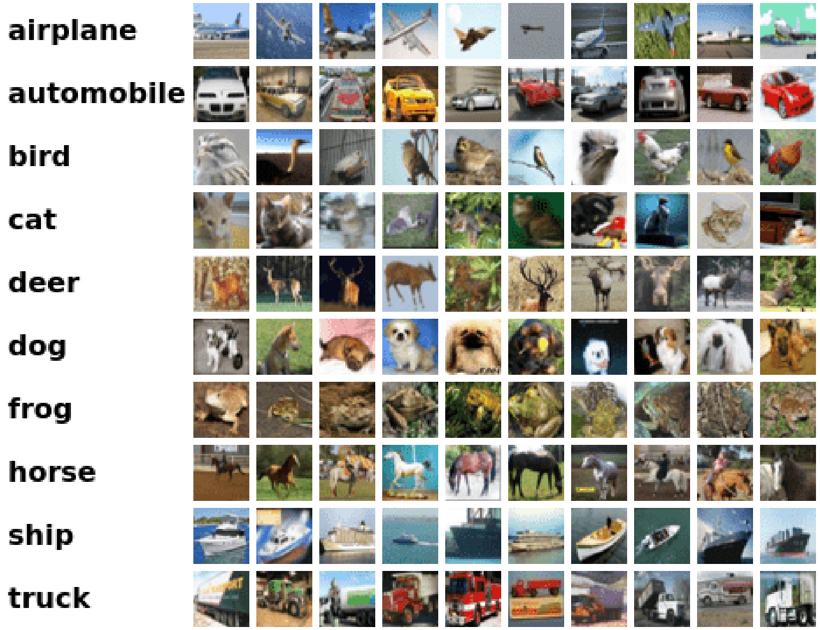
14: `/* Update parameters */`
15: Compute gradients and update

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \frac{\gamma}{B} \sum_{b=1}^{B} y_{i_b} g_{\sigma(\pi^{-1}(b))} \nabla_{\boldsymbol{\theta}} f_{\boldsymbol{\theta}}(\mathbf{x}_{i_b})$$

16: **end for**
17: **Return** the estimated $\boldsymbol{\theta}$

Experiments

CIFAR

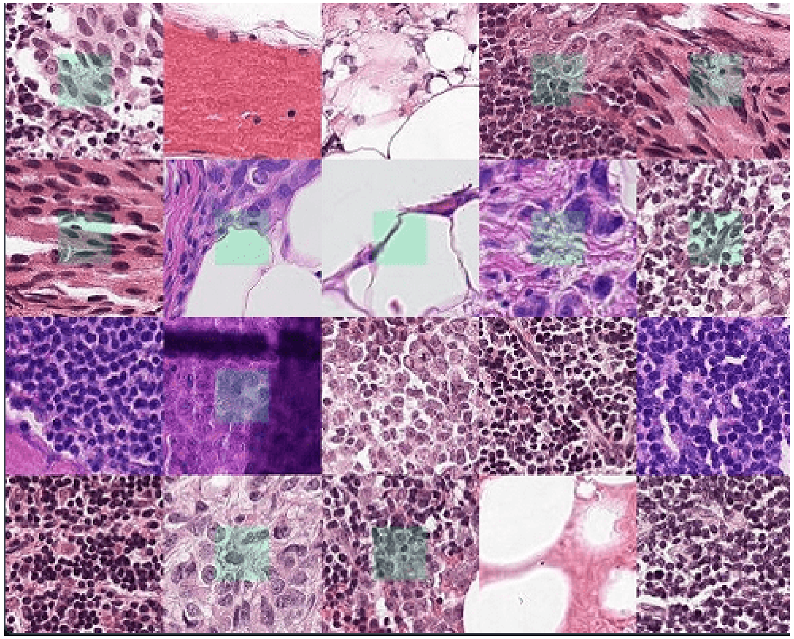


We construct binary CIFAR (CIFAR2), by selecting all possible pairs from CIFAR10, resulting:

10 x 9 / 2 = 45

CIFAR2 datasets.

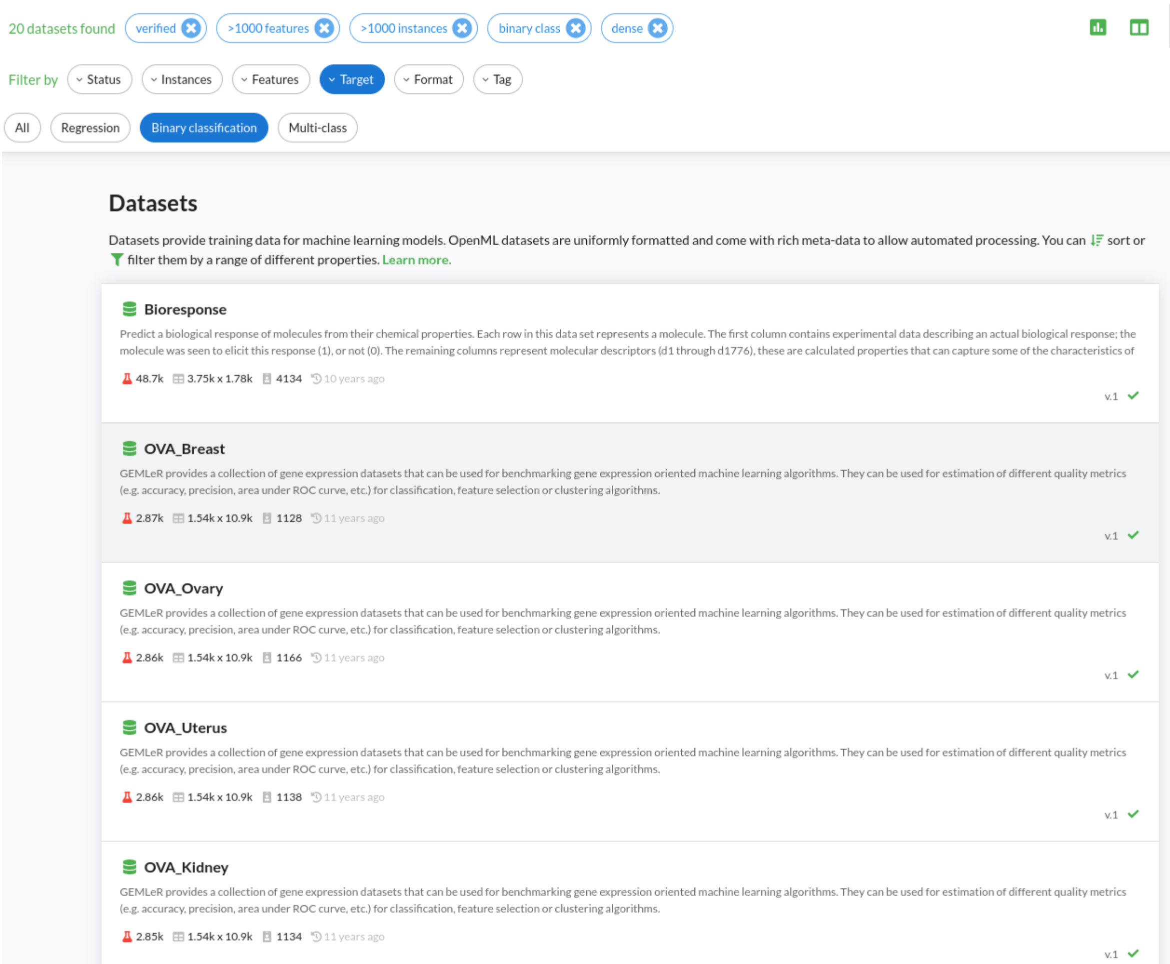
PCam



PCam is a binary image classification dataset comprising 327,680 96x96 images from histopathologic scans of lymph node sections

Experiments

OpenML



We applied a filering:

$n >= 1000$
$d >= 1000$
at least one official run

resulting 14 datasets

EnsLoss is a more desirable option compared to fixed losses in image data; and it is a viable option worth considering in tabular data.

PCam

Models	BCE	Exp	Hinge	EnsLoss
(Acc)				
ResNet34	76.91(0.52)	73.78(0.52)	77.20(0.18)	**82.33(0.30)**
ResNet50	77.23(0.51)	74.10(0.49)	77.96(0.34)	**82.00(0.07)**
VGG16	80.97(0.25)	77.11(0.50)	82.69(0.30)	**85.77(0.35)**
VGG19	81.58(0.25)	76.13(0.35)	82.77(0.41)	**85.91(0.19)**
(AUC)				
ResNet34	88.69(0.34)	83.30(0.57)	76.11(0.37)	**92.24(0.13)**
ResNet50	88.75(0.30)	83.51(0.46)	77.24(0.67)	**92.07(0.49)**
VGG16	93.35(0.26)	88.77(0.59)	86.18(0.56)	**95.44(0.24)**
VGG19	93.49(0.17)	87.89(0.46)	84.09(0.60)	**95.51(0.14)**

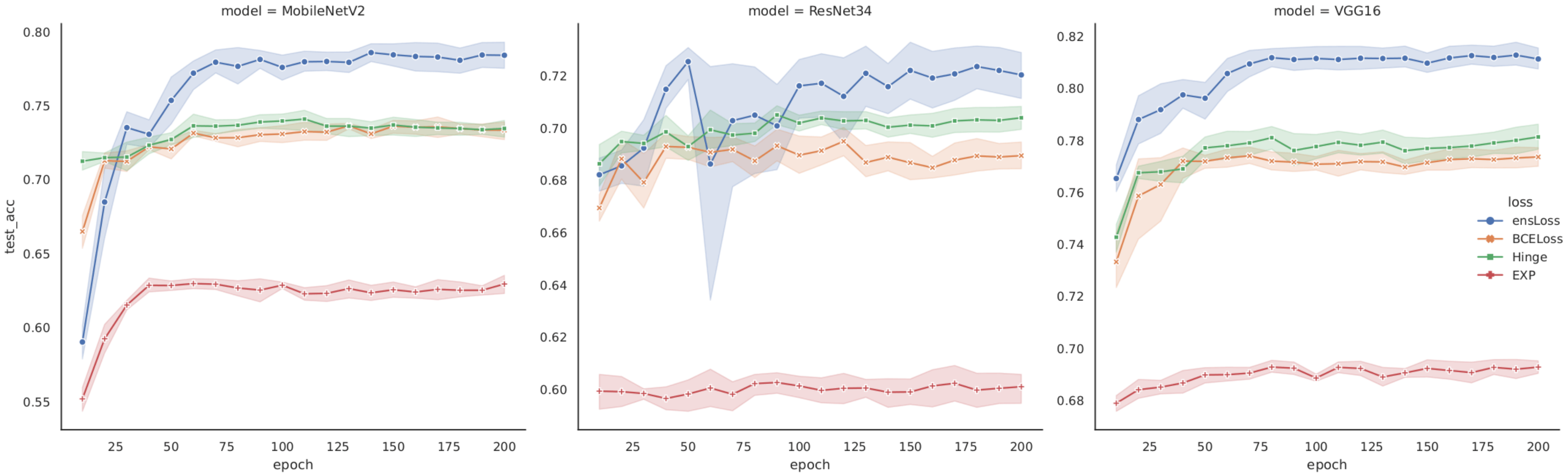
CIFAR2

(EnsLoss) Models	(vs BCE)	(vs Exp)	(vs Hinge)
	(better, no diff, worse) with $p < 0.05$		
ResNet34	(41, 4, 0)	(45, 0, 0)	(36, 9, 0)
ResNet50	(42, 3, 0)	(45, 0, 0)	(43, 2, 0)
ResNet101	(39, 6, 0)	(45, 0, 0)	(40, 5, 0)
VGG16	(36, 9, 0)	(45, 0, 0)	(29, 16, 0)
VGG19	(36, 9, 0)	(45, 0, 0)	(27, 18, 0)
MobileNet	(45, 0, 0)	(45, 0, 0)	(44, 1, 0)
MobileNetV2	(45, 0, 0)	(45, 0, 0)	(45, 0, 0)

OpenML

(EnsLoss) Models	(vs BCE)	(vs Exp)	(vs Hinge)
	(better, no diff, worse) with $p < 0.05$		
MLP(1)	(9, 4, 1)	(7, 5, 2)	(5, 4, 5)
MLP(3)	(7, 7, 0)	(8, 5, 1)	(9, 3, 2)
MLP(5)	(11, 3, 0)	(11, 2, 1)	(13, 0, 1)

Epoch-level performance



Compatibility of prevent-overfitting methods

REG	HP	BCE	EXP	HINGE	ENSLOSS
NO REG; baseline	—	67.99(0.30)	60.09(0.19)	68.19(0.40)	69.52(1.38)
WEIGHTD	5e-5	67.64(0.14)	60.43(0.23)	68.26(0.65)	71.01(1.04)
	5e-4	67.59(0.35)	61.57(0.56)	67.57(0.28)	**72.04(0.35)**
	5e-3	68.00(0.31)	62.26(0.45)	68.26(0.35)	70.84(0.67)
DROPOUT	0.1	67.50(0.39)	60.70(0.34)	67.89(0.30)	**72.48(0.22)**
	0.2	68.13(0.54)	60.02(0.52)	67.78(0.44)	70.08(1.28)
	0.3	67.65(0.29)	59.70(0.46)	67.78(0.49)	72.44(0.68)
DATAAUG	—	79.22(0.12)	58.96(0.31)	80.47(0.26)	**83.00(0.25)**

EnsLoss consistently outperforms the fixed losses across epochs;

and it is compatible with other methods, and their combination yields additional improvement.

Summary

The primary motivation of **EnsLoss** behind consists of two components: "**ensemble**" and the "**CC**" of the loss functions.

This concept can be extensively applied to various ML problems, by identify the *specific conditions for loss consistency* or calibration.

Thank you!