Rethinking Early Stopping: Refine, Then Calibrate

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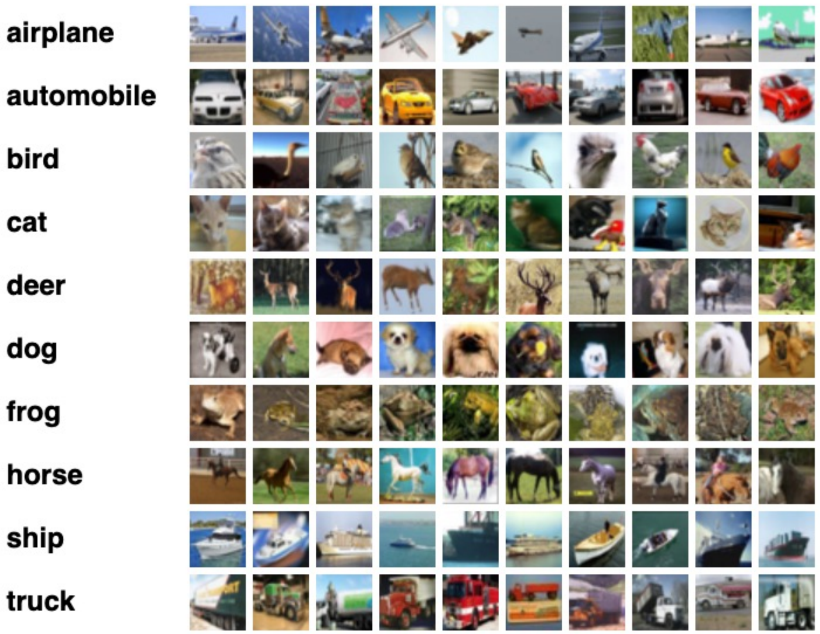
Outline

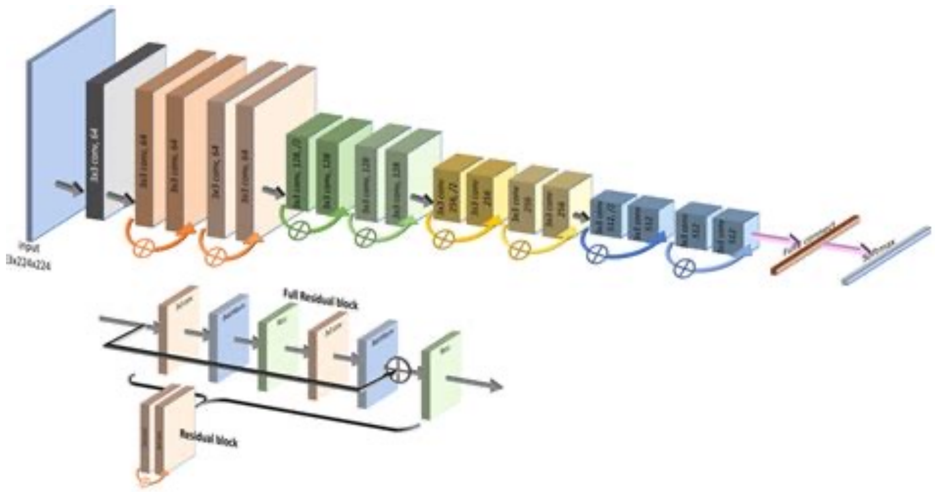
- Motivating example
- Loss function decomposition in classification
- Proposed method
- Empirical results
- A theoretical analysis: logistic regression in the high dimensional gaussian data model

Motivating example

Dataset D
Images, tabular, text…



Machine learning classifier f
logistic regression, boosted trees, neural net…



Probabilistic Predictions

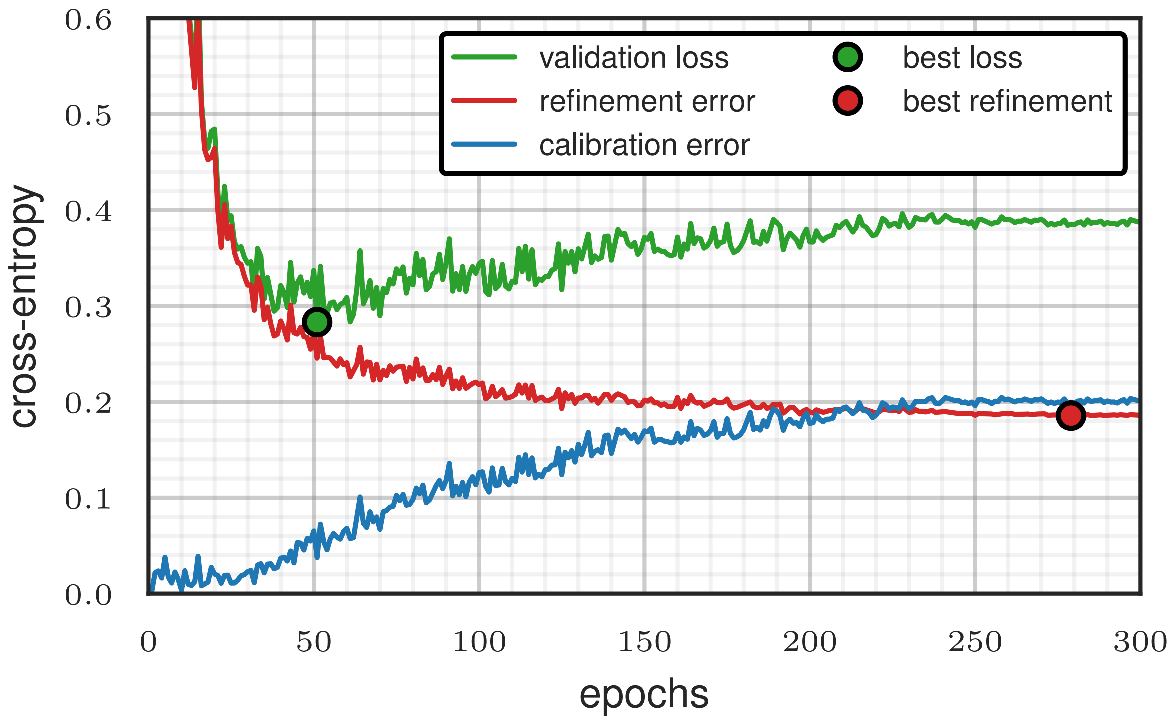
0.02	airplane
0.9	automobile
0.	bird
0.005	cat
0.	deer
0.005	dog
0.	frog
0.	horse
0.02	ship
0.05	truck

Motivating example

Model fitting

training, hyper-parameter search...

$$\min_{f \in \mathcal{F}} \mathrm{Risk}_D(f)$$



Training a ResNet-18 on CIFAR-10. We plot the cross-entropy loss on the validation set, with its calibration and refinement error terms.

What is this decomposition?

Is there a better way to train classifiers?

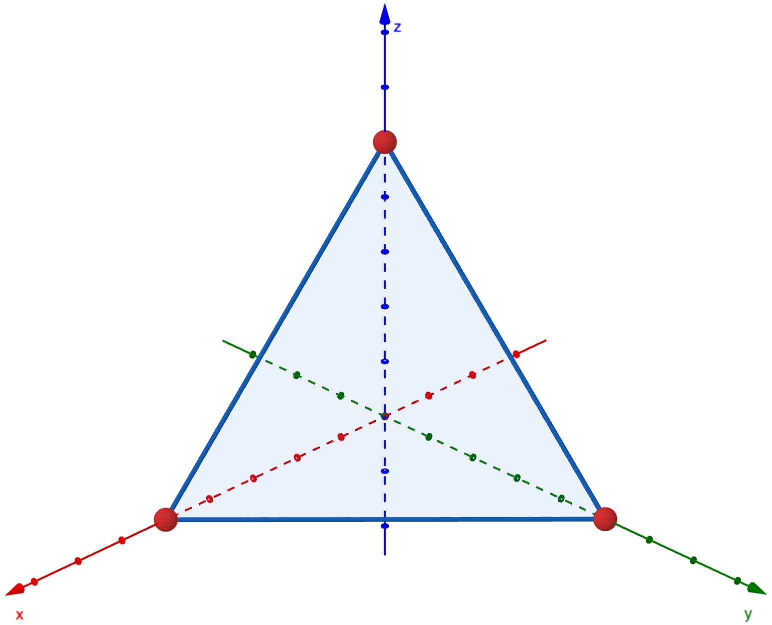
Proper loss functions in classification

Predictions in $\Delta_k = \{p \in [0,1]^k | \mathbf{1}^\top p = 1\}$, labels in $\mathcal{Y}_k = \{y \in \{0,1\}^k | \mathbf{1}^\top y = 1\}$.

Evaluated with loss functions $\ell : \Delta_k \times \mathcal{Y}_k \to \mathbb{R}_+$,

such as:

- The Brier score $\ell(p, y) = \|y - p\|_2^2$
- The log-loss $\ell(p, y) = -\sum_{i=1}^{k} y_i \log(p_i)$



The probability simplex (blue triangle) and label space (red dots) for k=3.

We overload the notation: $\ell(p, q) = \mathbb{E}_{y \sim q}[\ell(p, y)]$

A natural requirement is that $\ell(q, q) \leq \ell(p, q), \forall p, q$.

Then, ℓ is called proper (**log-loss and brier are proper losses**).

Gneiting, T., & Raftery, A. E. Strictly Proper Scoring Rules, Prediction, and Estimation. *Journal of the American Statistical Association.* 2007

Decomposition of proper losses

In machine learning, we usually have $(X, Y) \sim \mathcal{D}$.

We make predictions $p = f(X)$ with a model $f : \mathcal{X} \to \Delta_k$.

In this setting, for any proper loss,

$$\mathrm{Risk}_{\mathcal{D}}(f) = \mathbb{E}_{\mathcal{D}}[\ell(f(X), Y)] = \mathbb{E}_{\mathcal{D}}[d_\ell(f(X), C)] + \mathbb{E}_{\mathcal{D}}[e_\ell(C)]$$

with $\underbrace{d_\ell(p, q) = \ell(p, q) - \ell(q, q)}_{\ell\text{-divergence}}$, $\underbrace{e_\ell(q) = \ell(q, q)}_{\ell\text{-entropy}}$, and $\underbrace{C = \mathbb{E}_{\mathcal{D}}[Y | f(X)]}_{\text{Calibrated scores}}$.

Bröcker, J. Reliability, sufficiency, and the decomposition of proper scores. *Quarterly Journal of the Royal Meteorological Society.* 2009.

Kull, M., & Flach, P. Novel decompositions of proper scoring rules for classification: Score adjustment as precursor to calibration. *MLKDD.* 2015

Decomposition of proper losses

$$\underbrace{\mathbb{E}_{\mathcal{D}}[\ell(f(X),Y)]}_{\text{Risk}} = \underbrace{\mathbb{E}_{\mathcal{D}}[d_\ell(f(X),C)]}_{\text{Calibration error}} + \underbrace{\mathbb{E}_{\mathcal{D}}[e_\ell(C)]}_{\text{Refinement error}}$$

Risk: How good are my predictions?

=

Calibration error: is my model over/under confident?

+

Refinement error: how well does my model separates classes? (accuracy, AUROC)

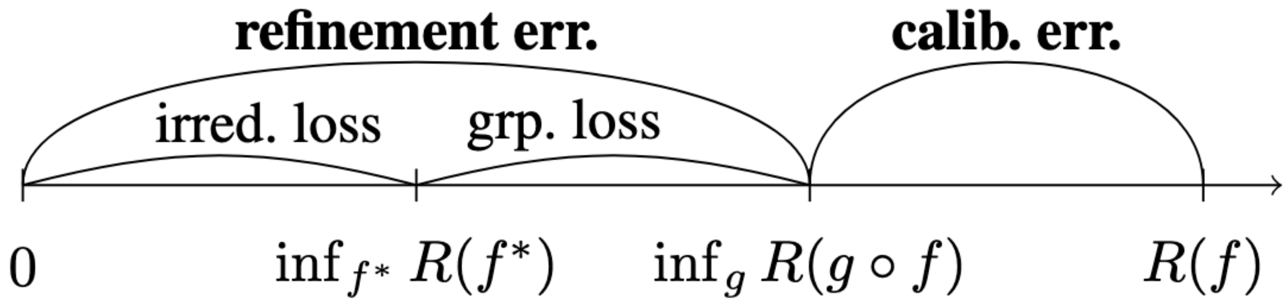
Proper loss ℓ	Divergence d_ℓ	Entropy e_ℓ
Logloss $-\sum_i y_i \log(p_i)$	KL divergence $\sum_i q_i \log \frac{q_i}{p_i}$	Shannon entropy $-\sum_i q_i \log q_i$
Brier score $\|y-p\|_2^2$	Squared distance $\|p-q\|_2^2$	Gini index $\sum_i q_i(1-q_i)$

A new variational decomposition

Theorem: Refinement error: $\mathcal{R}_\ell(f) = \min_g \mathrm{Risk}_\mathcal{D}(g \circ f)$

Calibration error: $\mathcal{K}_\ell(f) = \mathrm{Risk}_\mathcal{D}(f) - \min_g \mathrm{Risk}_\mathcal{D}(g \circ f)$

Optimal re-mapping: $g^*(f(X)) = \mathbb{E}_\mathcal{D}[Y | f(X)]$



Calibration in the ML literature

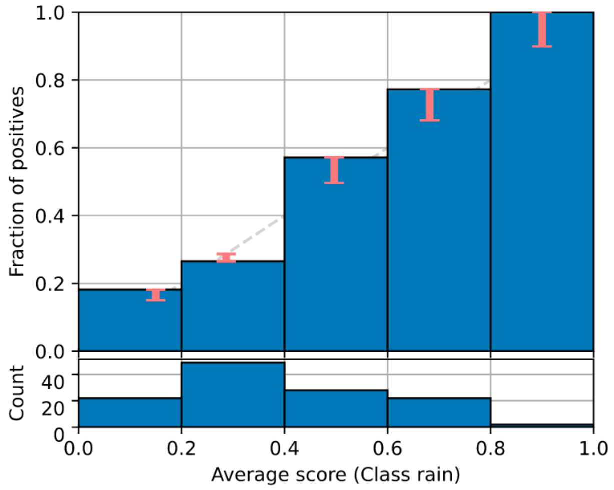
$$\mathbb{E}_{\mathcal{D}}[d(f(X), \mathbb{E}[Y|f(X)])]$$

Finite set D

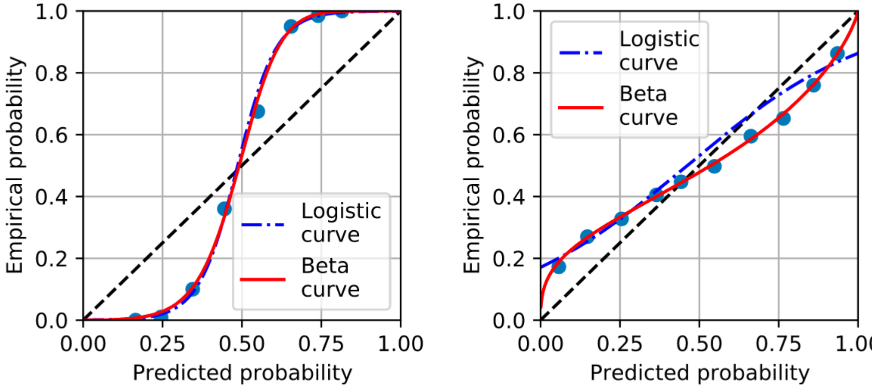
L_1

Binning

- Biased, Inconsistent
- Parameter dependent
- Multiclass?



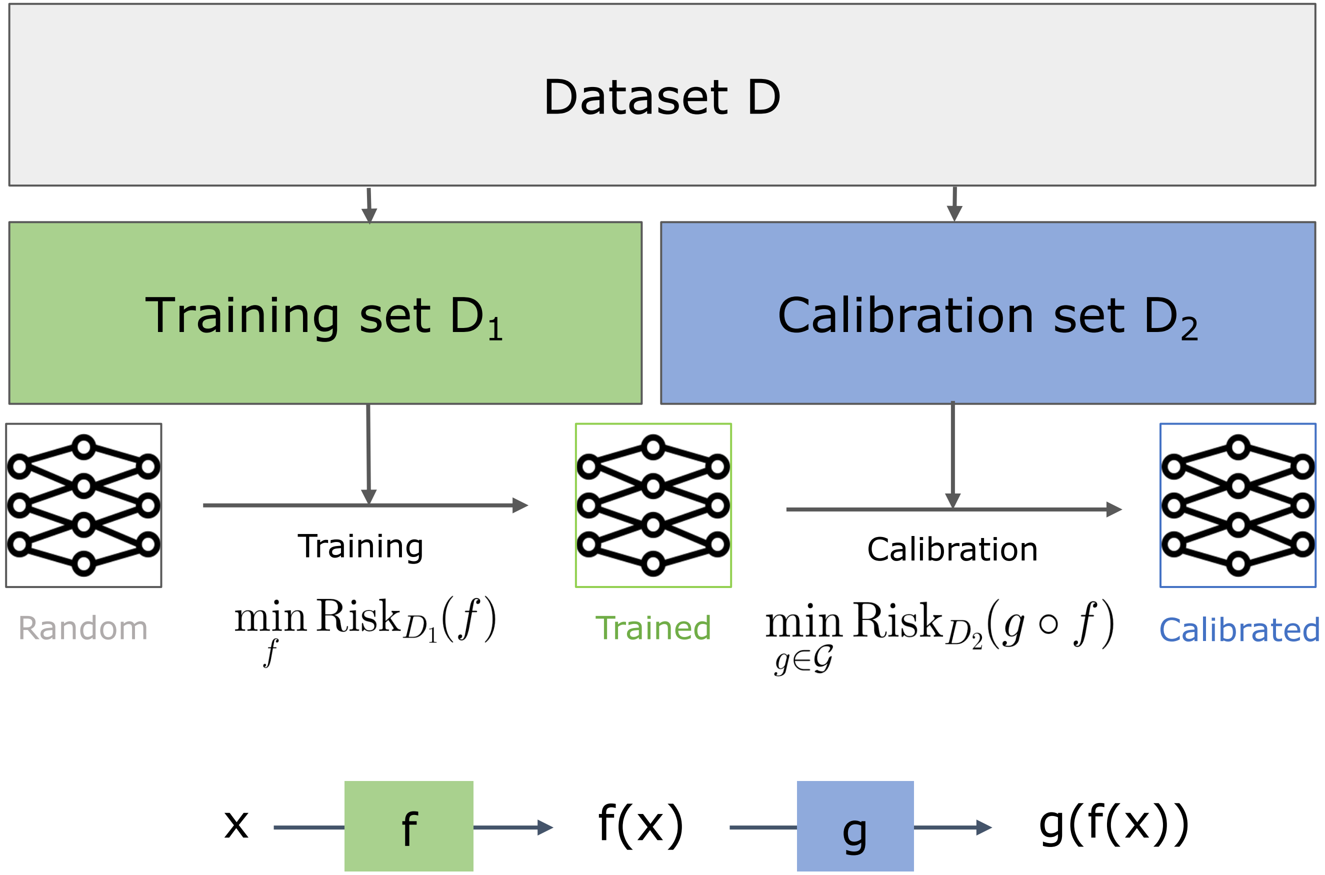
Post-hoc calibration:



(a) Underconfidence (b) Overconfidence

Silva Filho, Telmo, et al. Classifier calibration: a survey on how to assess and improve predicted class probabilities. *Machine Learning, 2023.*

Post-hoc calibration



Post-hoc calibration

Isotonic regression

$$\min_{g \nearrow} \mathrm{Risk}_{D_2}(g \circ f)$$

✅ Preserves the ROC convex hull.
✅ Theoretical guarantees.
❌ Ill defined in the multi-class case.

Temperature scaling

$$\min_{\alpha \in \mathbb{R}} \mathrm{Risk}_{D_2}(g_\alpha \circ f)$$

Where $g_\alpha(p) = \mathrm{Softmax}(\alpha \log(p))$

✅ Preserves refinement error.
✅ Inherently multi-class.
❌ No theoretical guarantees?

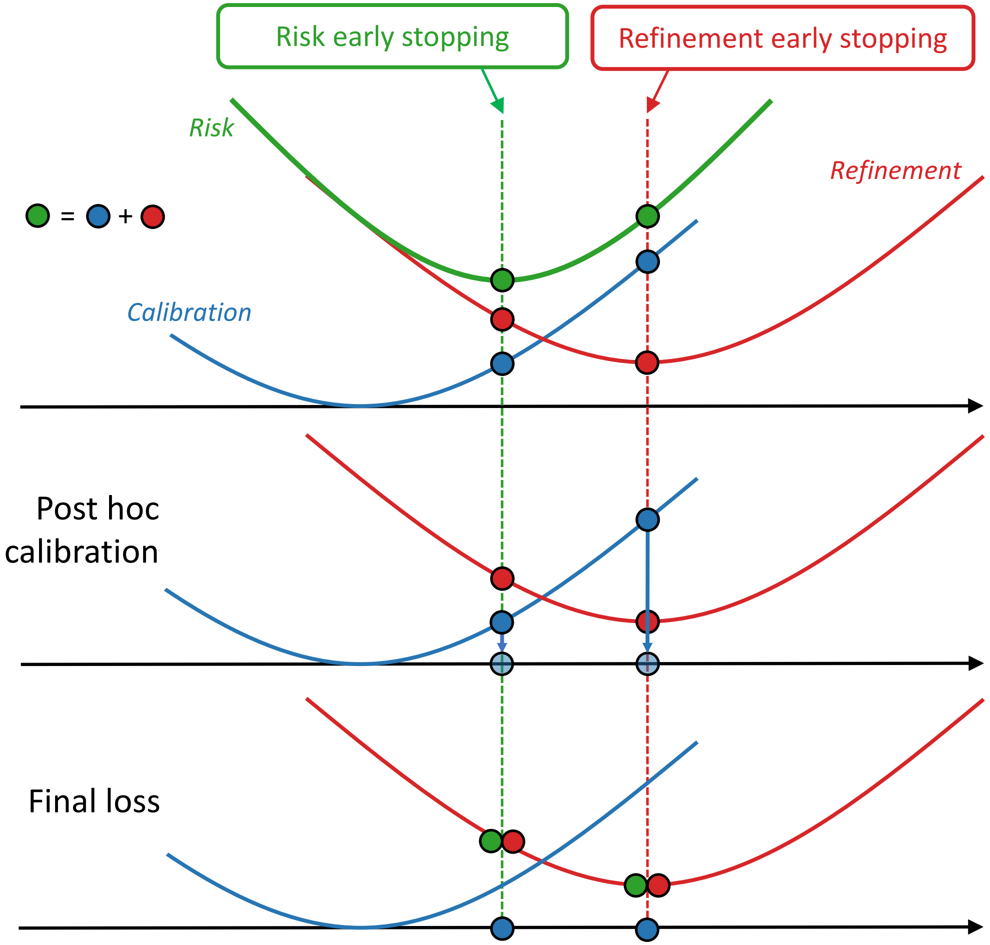
Zadrozny, B. & Elkan, C. Transforming classifier scores into accurate multiclass probability estimates. *International conference on Knowledge discovery and data mining*. 2002.

Berta, E., Bach, F. & Jordan, M. Classifier Calibration with ROC-Regularized Isotonic Regression. *International Conference on Artificial Intelligence and Statistics.* 2024.

Guo, C., Pleiss, G., Sun, Y., & Weinberger, K. Q. On calibration of modern neural networks. *International conference on machine learning*. 2017.

Our method: Refine, Then Calibrate

Early stopping	Training minimizes	Post hoc minimizes
Risk	Cal. + Ref.	Cal.
Refinement	Ref.	Cal.



How can we estimate refinement?

Using validation accuracy? Area under the ROC curve?

Refinement with our variational reformulation — Validation loss after post-hoc calibration.

$$\underbrace{\mathcal{R}_\ell(f) = \min_g \mathrm{Risk}_{\mathcal{D}}(g \circ f)}_{\text{Refinement with our variational reformulation}} \simeq \underbrace{\min_{g \in \mathcal{G}} \mathrm{Risk}_{D_2}(g \circ f)}_{\text{Validation loss after post-hoc calibration.}}$$

Choosing the set $\mathcal{G}$

Large $\mathcal{G}$?
e.g. Isotonic regression

- ✅ little bias in our estimator
- ❌ over-fitting the validation set D_2

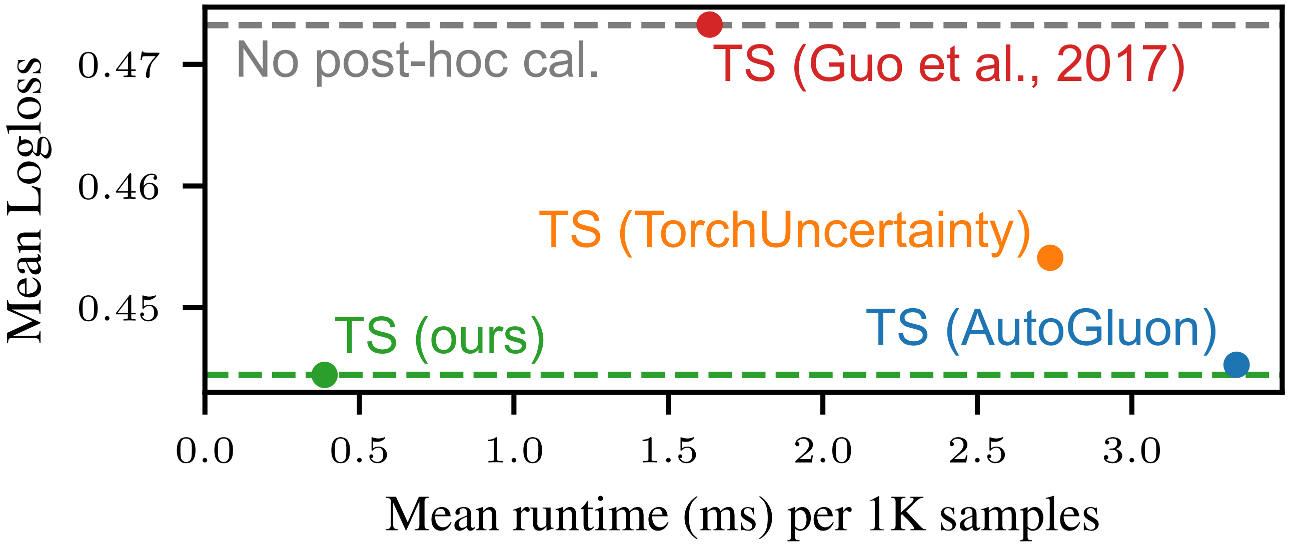
Small $\mathcal{G}$?
e.g. Temperature scaling

- ✅ robust to over-fitting
- ❌ biased estimator? Unless close to $g^*(f(X)) = \mathbb{E}_{\mathcal{D}}[Y|f(X)]$

We evaluate **TS-refinement** = validation loss after temperature scaling

⚠️ Could be any other refinement estimator.

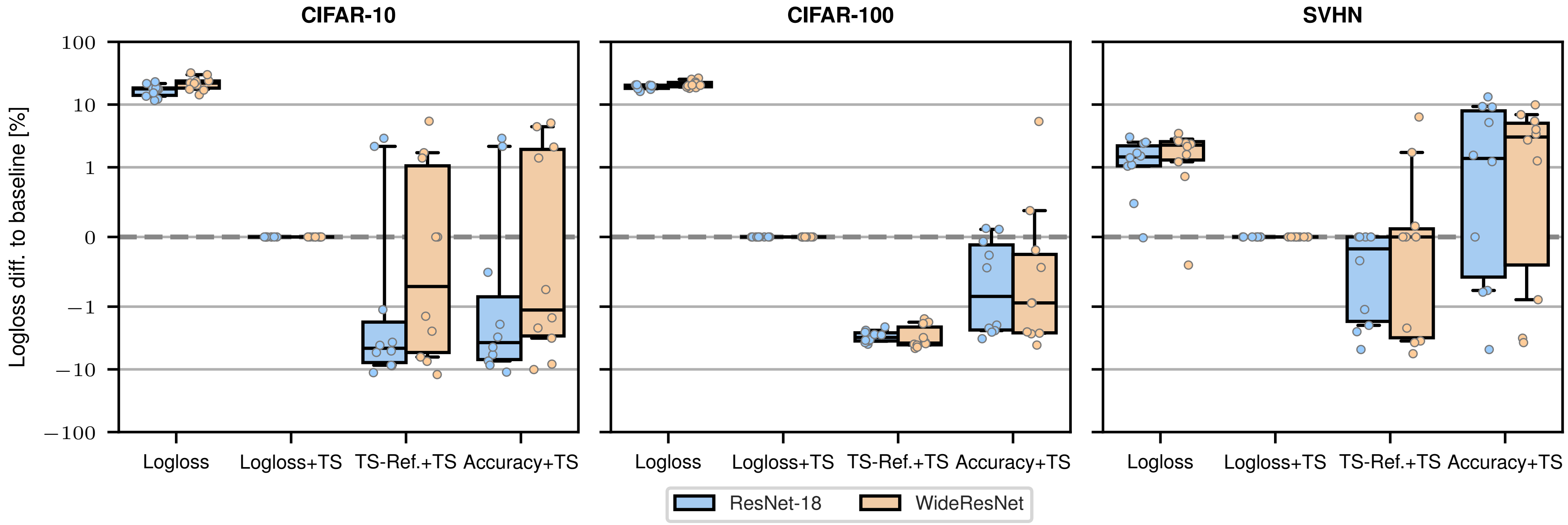
Use the best implementation, ours!



Runtime versus mean benchmark scores of different TS implementations.
Runtimes are averaged over validation sets with 10K+ samples. Evaluation is on XGBoost models trained with default parameters, using the epoch with the best validation accuracy.

github.com/dholzmueller/probmetrics

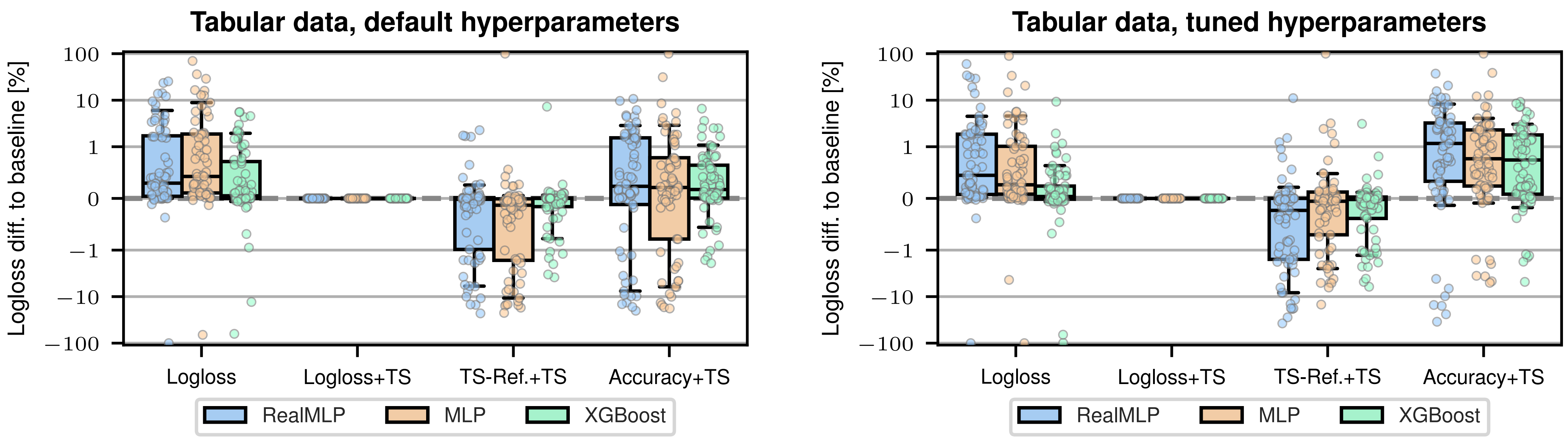
Results – computer vision



Relative differences in test log-loss (lower is better) between logloss+TS and other procedures on vision datasets.
"+TS" indicates temperature scaling applied to the final model. Each dot represents a training run on one dataset. Box-plots show the 10%, 25%, 50%, 75%, and 90% quantiles. Relative differences (y-axis) are plotted using a log scale.

github.com/eugeneberta/RefineThenCalibrate-Vision

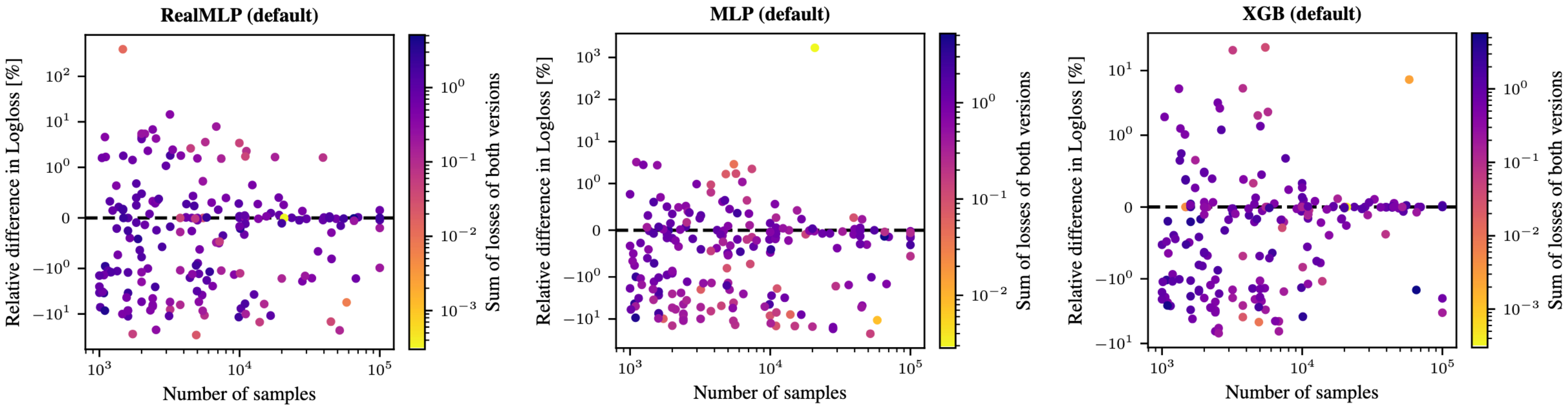
Results – tabular data



Relative differences in test logloss (lower is better) between logloss+TS and other procedures on tabular datasets.
"+TS" indicates temperature scaling applied to the final model. Each dot represents one dataset with 10K+ samples. Percentages are clipped to [−100, 100] due to one outlier with almost zero loss. Box-plots show the 10%, 25%, 50%, 75%, and 90% quantiles. Relative differences (y-axis) are plotted using a log scale.

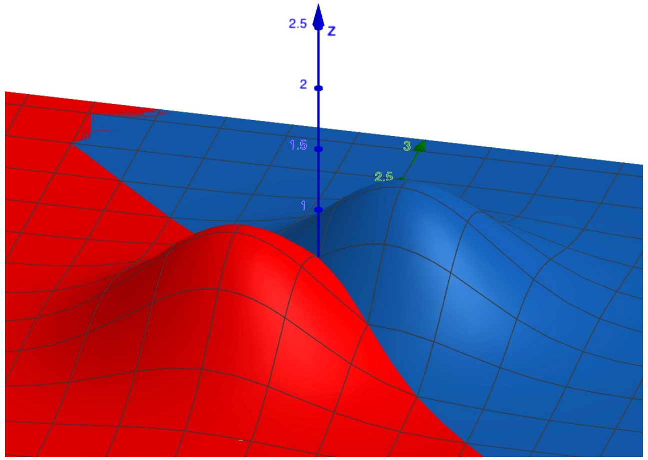
github.com/dholzmueller/pytabkit

Results – effect of validation set size



Relative differences in logloss of using TS-Refinement vs. logloss for selecting the best epoch with default hyperparameters.
Each method applies temperature scaling on the final model. Each dot represents one dataset. Values below zero mean that TS-refinement performs better. A light color indicates datasets where methods achieve very low loss.

Theoretical analysis: the Gaussian data model



Gaussian data model:

$$X \in \mathbb{R}^p, Y \in \{-1, 1\} \quad \begin{cases} X \sim \mathcal{N}(\mu, \Sigma) \text{ if } Y = 1 \\ X \sim \mathcal{N}(-\mu, \Sigma) \text{ if } Y = -1 \end{cases}$$

Linear classifier:

$$f(X) = \sigma(w^\top X) \qquad \text{with} \qquad \sigma(x) = \frac{1}{1 + \exp(-x)}$$

In this well studied setting, $w^* = 2\Sigma^{-1}\mu$

Theoretical analysis: the Gaussian data model

The error rate writes $\mathrm{err}(w) = \Phi(-a_w/2)$ with, $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-\frac{t^2}{2}) dt$

And $\underbrace{a_w = \frac{\langle w, w^* \rangle_\Sigma}{\|w\|_\Sigma}}_{\text{Expertise level}}$ with $\underbrace{\|w\|_\Sigma = \sqrt{w^\top \Sigma w}}_{\text{Confidence level}}$, $\langle w, w^* \rangle_\Sigma = w^\top \Sigma w^*$

Theorem 5.1. *For proper loss ℓ, the calibration and refinement errors of our model are*

$$\mathcal{K}_\ell(w) = \mathbb{E}\Big[d_\ell\Big(\sigma\Big(\|w\|_\Sigma\Big(z + \frac{a_w}{2}\Big)\Big), \sigma\Big(a_w\Big(z + \frac{a_w}{2}\Big)\Big)\Big)\Big]$$
$$\mathcal{R}_\ell(w) = \mathbb{E}\Big[e_\ell\Big(\sigma\Big(a_w\Big(z + \frac{a_w}{2}\Big)\Big)\Big)\Big],$$

where the expectation is taken on $z \sim \mathcal{N}(0, 1)$.

Theorem 5.2. *The re-scaled weight vector $w_s \leftarrow sw$ with $s = \langle w, w^* \rangle_\Sigma / \|w\|_\Sigma^2$ yields null calibration error $\mathcal{K}(w_s) = 0$ while preserving the refinement error $\mathcal{R}(w_s) = \mathcal{R}(w)$.*

Theoretical analysis: regularized logistic regression in high dimension

The weight vector learned with regularized logistic regression:

$$\min_{w \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-y_i w^\top X_i)) + \frac{\lambda}{2} \|w\|^2$$

Has the following distr. when $n, p \to \infty$ with a constant ratio,

$$w_\lambda \sim \mathcal{N}\left(\eta(\lambda I_p + \tau\Sigma)^{-1}\mu, \frac{\gamma}{n}(\lambda I_p + \tau\Sigma)^{-1}\Sigma(\lambda I_p + \tau\Sigma)^{-1}\right)$$

Proposition 6.1. *For $n, p \to \infty$,*

$$\langle w_\lambda, w^* \rangle_\Sigma \xrightarrow{P} \mathbb{E}_{\sigma \sim F}\left[\frac{2\eta c^2}{\lambda + \tau\sigma}\right],$$

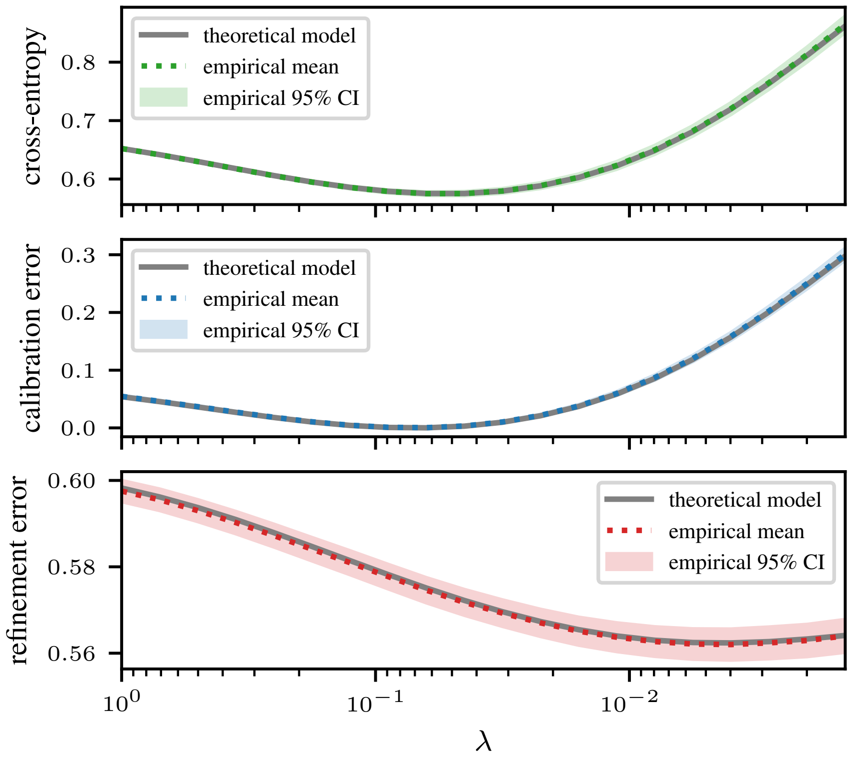
$$\|w_\lambda\|_\Sigma^2 \xrightarrow{P} \mathbb{E}_{\sigma \sim F}\left[\frac{\gamma r \sigma^2 + \eta^2 c^2 \sigma}{(\lambda + \tau\sigma)^2}\right],$$

where the convergence is in probability.

Mai, X., Liao, Z., & Couillet, R. A large scale analysis of logistic regression: Asymptotic performance and new insights. *International Conference on Acoustics, Speech and Signal Processing.* 2019.

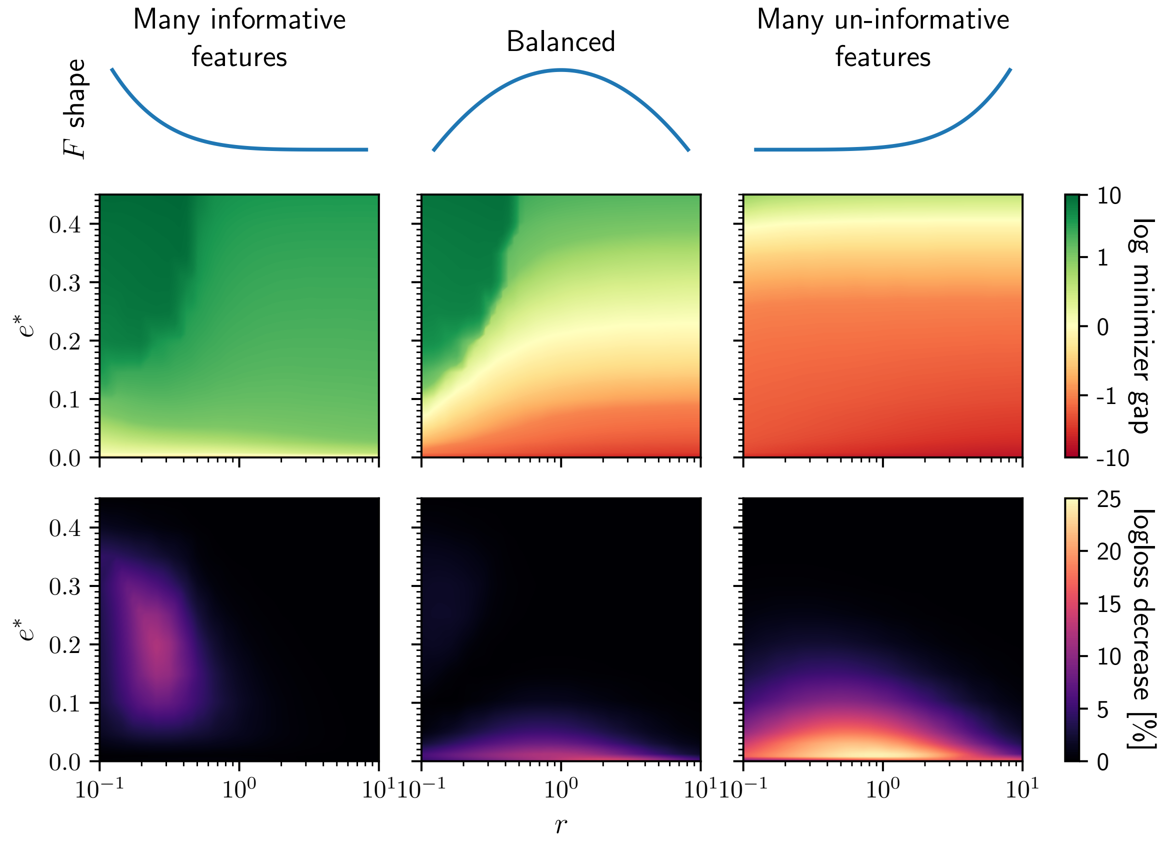
Theoretical analysis: regularized logistic regression in high dimension

We provide an efficient solver to compute cal. and ref. errors under our mathematical model: github.com/eugeneberta/RefineThenCalibrate-Theory



Cross-entropy, calibration and refinement errors when λ varies. The spectral distribution F is uniform, $e_* = 10\%$, $r = 1/2$. We fit a logistic regression on 2000 random samples from our data model, we compute the resulting calibration and refinement errors and plot 95% error bars after 50 seeds.

Theoretical analysis: regularized logistic regression in high dimension



Influence of problem parameters on calibration and refinement minimizers. *First row: spectral distribution shape. Second row: log gap between the two minimizers. In green regions, calibration is minimized earlier, while in red regions it is refinement. Third row: relative logloss gain (%) obtained with refinement early stopping.*

Thanks for listening!

Read the full paper:

Use our method on your favorite classification task: