

PAC Confidence Predictions for Deep Neural Network Classifier

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Quantifying Uncertainty of Deep Neural Network Predictions



Source: Mask RCNN

✓ Accurate label predictions

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How to predict confidences with finite sample guarantees?

PAC Calibration

PAC calibration: The goal of PAC calibration is to find a confidence coverage predictor \hat{C} such that it contains true confidence with high probability—*i.e.*,

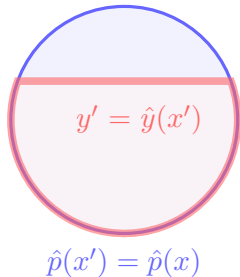
$$(\text{true confidence}) \in \hat{C}(x; \hat{f})$$

Here, a pretrained predictor \hat{f} is given.

True Confidence

True confidence on x associated with \hat{f} (due to the known calibration definition [DeGroot and Fienberg, 1983, Zadrozny and Elkan, 2002, Park et al., 2020]):

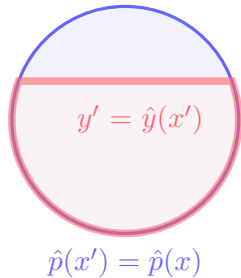
$$c_{\hat{f}}^*(x) := \mathbb{P}_{(x', y') \sim D} [y' = \hat{y}(x') \mid \hat{p}(x') = \hat{p}(x)]$$



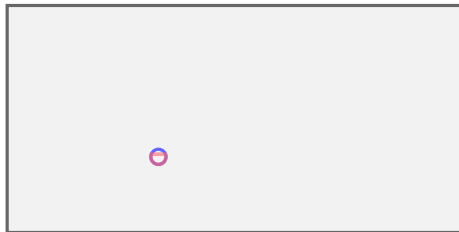
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sample space Ω

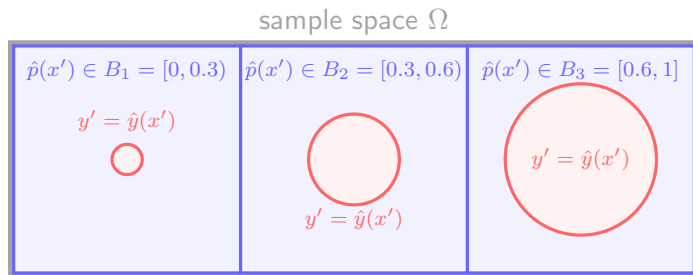


Estimating the true confidence with finite samples is challenging

“Coarsen” True Confidence

$$c_{\hat{f}}(x) := \mathbb{P}_{(x', y') \sim D} \left[y' = \hat{y}(x') \mid \hat{p}(x') \in B_{\kappa_{\hat{f}}(x)} \right]$$

- $\kappa_{\hat{f}} : \mathcal{X} \rightarrow \{1, 2, \dots, K\}$: the index of the bin for x —i.e., $\hat{p}(x) \in B_{\kappa_{\hat{f}}(x)}$



PAC Calibration

Definition

Given $\delta \in \mathbb{R}_{>0}$ and $n \in \mathbb{N}$, \hat{C} is *probably approximately correct (PAC)* if for all D

$$\overbrace{c_{\hat{f}}(x) \in \hat{C}(x; \hat{f}, Z_n)}^{\text{approximately correct}}$$

For a formal connection to the PAC learning theory, see Appendix A.

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Problem

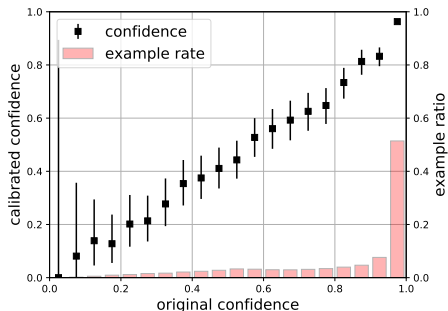
Find a PAC confidence coverage predictor \hat{C} , while ensuring its size is small.

Our Approach

Main idea: Coarsened true confidence is the parameter of a Binomial distribution

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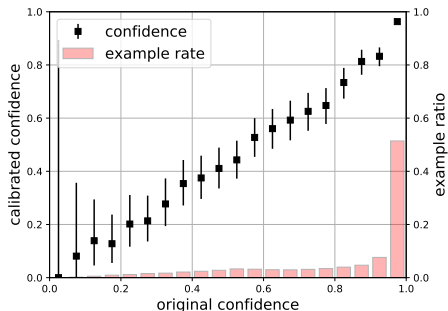
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Pictorial representation of \hat{C}

Our Approach

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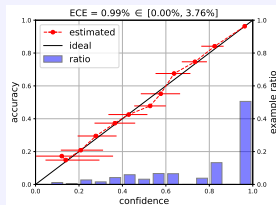
Pictorial representation of \hat{C}

Theorem

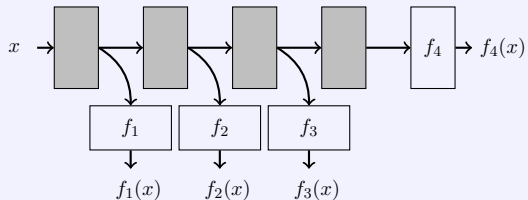
\hat{C} satisfies the PAC property.

Applications

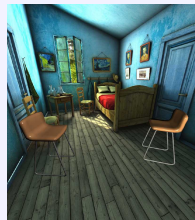
Classifier calibration



Fast DNN Inference

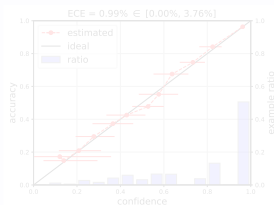


Safe Planning

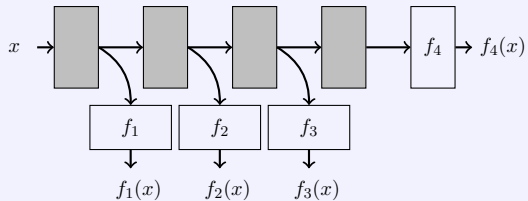


Applications

Classifier calibration



Fast DNN Inference



Safe Planning



Application: Fast DNN Inference

Motivation:

- AlexNet: fast but inaccurate (top-1 error: 43.45%)
- ResNet152: slow but accurate (top-1 error: 21.69%)

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Can we combine the two models to improve inference speed while maintaining high accuracy?

Model Composition

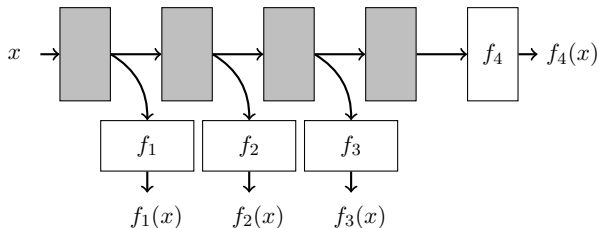


Figure: A composed model in a cascading way for $M = 4$.

Composed classifier:

$$\hat{y}_C(x; \gamma_{1:M-1}) := \begin{cases} \hat{y}_1(x) & \text{if } \hat{p}_1(x) \geq \gamma_1 \\ \hat{y}_2(x) & \text{if } \hat{p}_1(x) < \gamma_1 \wedge \hat{p}_2(x) \geq \gamma_2 \\ \vdots & \\ \hat{y}_{M-1}(x) & \text{if } \bigwedge_{m=1}^{M-2} (\hat{p}_m(x) < \gamma_m) \wedge \hat{p}_{M-1}(x) \geq \gamma_{M-1} \\ \hat{y}_M(x) & \text{otherwise,} \end{cases}$$

Our Approach

$$\begin{array}{ll} \min_{\gamma_{1:M-1}} & \text{(inference time)} \\ \text{subj. to} & p_{\text{error}} := \underbrace{\mathbb{P}_{(x,y) \sim D} [\hat{y}_C(x; \gamma_{1:M-1}) \neq y]}_{\text{error}_{\text{composed model}}} - \underbrace{\mathbb{P}_{(x,y) \sim D} [\hat{y}_M(x) \neq y]}_{\text{error}_{\text{slow model}}} \leq \xi. \end{array}$$

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Theorem

We have $p_{\text{error}} \leq \xi$ with probability at least $1 - \delta$ over $Z \sim D^n$.

Experiment: Comparison

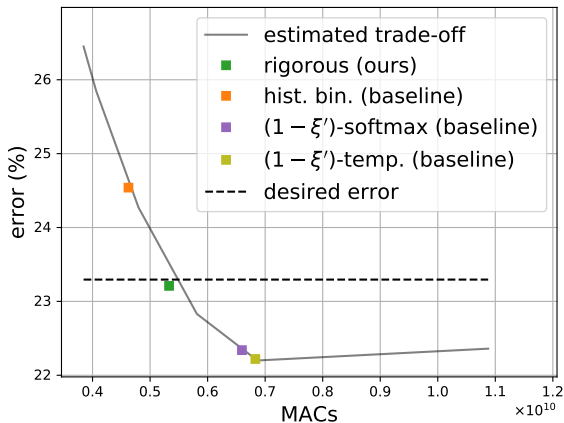


Figure: $M = 2$, $N = 20,000$, $\xi = 0.02$, $\delta = 10^{-2}$

- MACs: Multiplication ACcumulation operations

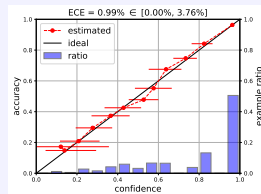
Conclusion

PAC Calibration Problem

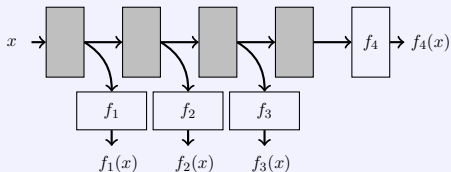
Approach: CP interval + hist. binning



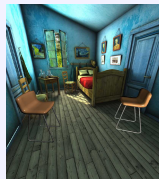
Application 1: Classifier Calibration



Application 2: Fast DNN Inference



Application 3: Safe Planning



Feel free to visit to our poster session if you have more questions!

References I

[DeGroot and Fienberg, 1983] DeGroot, M. H. and Fienberg, S. E. (1983).

The comparison and evaluation of forecasters.

Journal of the Royal Statistical Society: Series D (The Statistician), 32(1-2):12–22.

[Park et al., 2020] Park, S., Bastani, O., Weimer, J., and Lee, I. (2020).

Calibrated prediction with covariate shift via unsupervised domain adaptation.

In *The 23rd International Conference on Artificial Intelligence and Statistics*.

[Zadrozny and Elkan, 2002] Zadrozny, B. and Elkan, C. (2002).

Transforming classifier scores into accurate multiclass probability estimates.

In *Proceedings of the eighth ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 694–699. ACM.