T-Cal: An optimal test for the calibration of predictive models

Edgar Dobriban, University of Pennsylvania

based on joint work with
Donghwan Lee, Xinmeng Huang, and Hamed Hassani

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Overview

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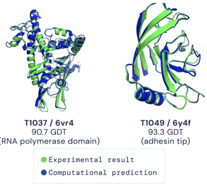

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: **After two days of intense debate, the United Methodist Church has agreed to a historic split - one that is expected to end in the creation of a new denomination, one that will be "theologically and socially conservative," according to The Washington Post. The majority of delegates attending the church's annual General Conference in May voted to strengthen a ban on the ordination of LGBTQ clergy and to write new rules that will "discipline" clergy who officiate at same-sex weddings. But those who opposed these measures have a new plan: They say they will form a separate denomination by 2020, calling their church the Christian Methodist denomination.**

Figure 3.14: The GPT-3 generated news article that humans had the greatest difficulty distinguishing from a human written article (accuracy: 12%).

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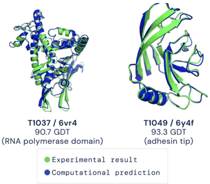

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- Meanwhile, growing concerns: safety, ethics, energy- and sample-efficiency, uncertainty

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- Examples of uncertainty:
  - GPT-3: given text prompt, ...?
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- Standard ML pipeline does not provide a solution

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  - Prediction Set: find mapping C of inputs to subsets of $\mathcal{Y}$: $P(y \in C(x)) \geqslant 1 - \alpha$, for some $\alpha \in (0, 1)$.

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- Example problems:
  - Prediction Set: find mapping C of inputs to subsets of $\mathcal{Y}$: $P(y \in C(x)) \geqslant 1 - \alpha$, for some $\alpha \in (0, 1)$.
  - Calibration: construct probability predictions that reflect true probabilities. For binary classification, for all appropriate z,

$$P(y = 1 | f(x) = z) \approx z$$

Uncertainty Quantification for ML - My course at Penn

github.com/dobriban/Topics-In-Modern-Statistical-Learning

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STAT 991: Topics In Modern Statistical Learning (UPenn, 2022 Spring)

This class surveys advanced topics in statistical learning based on student presentations.

The core topic of the course is uncertainty quantification for machine learning methods. While modern machine learning methods can have a high prediction accuracy in a variety of problems, it is still challenging to properly quantify their uncertainty. There has been a recent surge of work developing methods for this problem. It is one of the fastest developing areas in contemporary statistics. This course will survey a variety of different problems and approaches, such as calibration, prediction intervals (and sets), conformal inference, OOD detection, etc. We will discuss both empirically successful/popular methods as well as theoretically justified ones. See below for a sample of papers.

About

Materials for STAT 9911303: Topics In Modern Statistical Learning (UPenn, 2022 Spring) - focus on uncertainty quantification

machine-learning deep-learning prediction uncertainty-quantification conformal-prediction tolerance-intervals

Calibration

- Input $x \in \mathbb{R}^d$; output: one-hot encoded label $y \in \{0, 1\}^K$
- A probabilistic classifier (probability predictor) $f : \mathbb{R}^d \to \Delta_{K-1}$ (simplex of probability distributions over $1, \dots, K$) is calibrated if

$$P(\mathrm{y}_k = 1 | f(\mathrm{x}) = \mathrm{z}) = \mathrm{z}_k \quad \text{for any } k \in [K] = \{1, \dots, K\} \text{ and } z \in \Delta_{K-1}$$

Here $z_k = [f(x)]_k$

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- Often focus on top-1 calibration, condition on $f^+(x) = \max_k [f(x)]_k$; use

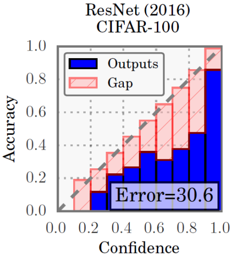
  $$y^+ = I(y = y_{\hat{k}(x)}), \quad \hat{k}(x) = \arg\max_k [f(x)]_k,$$

  so calibration amounts to correctly predicting accuracy

  $$P(y = y_{\hat{k}(x)} | f^+(x)) = f^+(x)$$

Calibration

- Modern finding: powerful ML methods (e.g., deep CNNs) are *over-confident* and *mis-calibrated*



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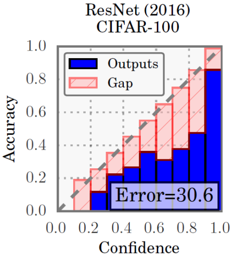

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- Historical context: Humans are *also over-confident*

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- Present day: ML community

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2. Test calibration
3. If it is mis-calibrated, retrain/re-calibrate

Testing Calibration

- Classical tests of calibration (Cox, Miller): Given $B_i \sim \text{Bernoulli}(q_i)$, $i = 1, \ldots, n$, test $q_i = p_i$, for a given probability predictions p_i.

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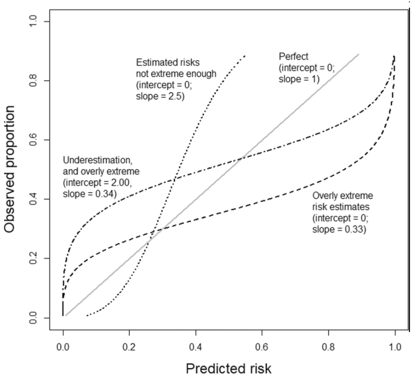

Figure: Van Calster et al, 2015

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- Further key questions: which test statistic? optimality?

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- Which test statistic? optimality?
  - Debiased plug-in estimator of Empirical Calibration Error (ECE)
  - Minimax optimal over Hölder smooth calibration curves

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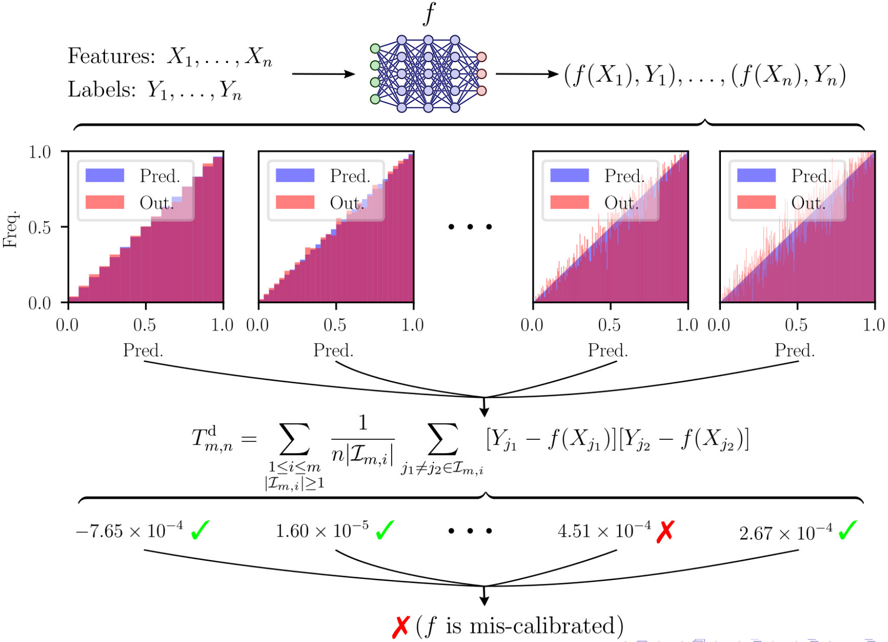

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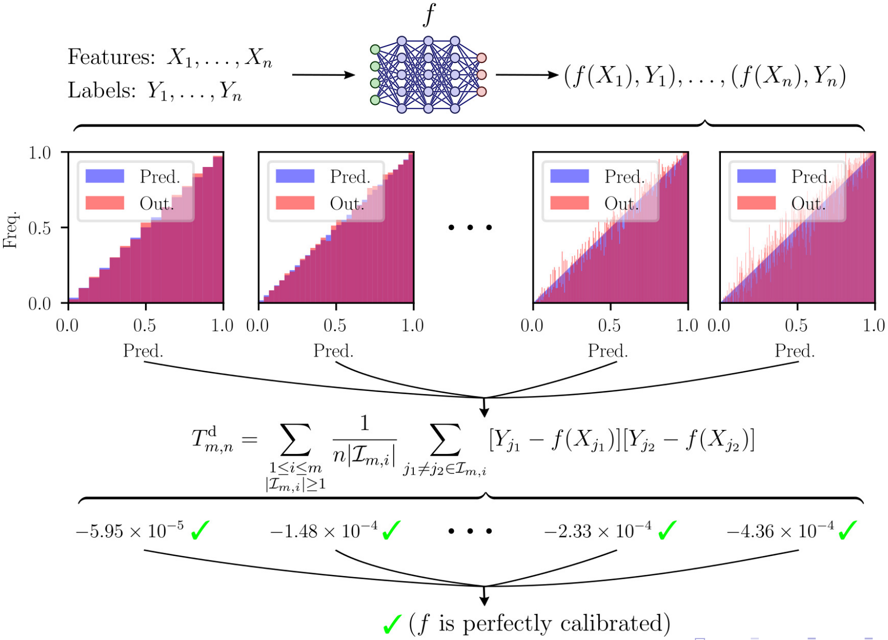

Overview

Regression/Residual Function

- Recall: A classifier (probability predictor) $f : \mathbb{R}^d \to \Delta_{K-1}$ is calibrated if

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- The calibration curve (*regression function*) $\mathrm{reg}_f : \Delta_{K-1} \to \Delta_{K-1}$ is

$$\mathrm{reg}_f(\mathrm{z}) := \mathbb{E}[Y \mid f(X) = \mathrm{z}].$$

  We define the *residual function* (mis-calibration curve) $\mathrm{res}_f : \Delta_{K-1} \to \mathbb{R}^K$ as

$$\mathrm{res}_f(\mathrm{z}) := \mathrm{reg}_f(\mathrm{z}) - \mathrm{z}.$$

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$$\mathrm{res}_f(\mathrm{z}) := \mathrm{reg}_f(\mathrm{z}) - \mathrm{z}.$$

- In this language, the classifier f is calibrated if

$$\mathrm{res}_f(Z) = 0,$$

  almost surely w.r.t. the law of $Z = f(X)$.

Expected Calibration Error

- For any $p \geq 1$, the ℓ_p-ECE is

$$\begin{aligned}\ell_p\text{-ECE}_P(f) =& \mathbb{E}_{Z \sim P_Z}\left[\|\mathrm{reg}_f(Z) - Z\|_p^p\right]^{\frac{1}{p}} \\ =& \mathbb{E}_{Z \sim P_Z}\left[\|\mathrm{res}_f(Z)\|_p^p\right]^{\frac{1}{p}}.\end{aligned}$$

- $\ell_p\text{-ECE}_P(f) = 0$ iff f is calibrated under P

Hypothesis Testing Setup

- $\mathcal{P}_{s,L,K}$: distributions over $(f(X), Y) = (Z, Y) \in \Delta_{K-1} \times \mathcal{Y}$ under which $\mathrm{z} \mapsto [\mathrm{res}_{f,P}(\mathrm{z})]_k$ is (s, L)-Hölder continuous[1] for every $k \in \{1, \dots, K\}$.

[1] for a Hölder smoothness parameter s and a Hölder constant L

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- Goal: Test the *null hypothesis* of calibration against the *alternative* of an ε-calibration error:

$$H_0 : P \in \mathcal{P}_0 \quad \text{versus} \quad H_1 : P \in \mathcal{P}_1(\varepsilon, p, s).$$

- Calibrated data distributions

$$\mathcal{P}_0 := \left\{P \in \mathcal{P}_{s,L,K} : \mathrm{res}_{f,P}(Z) = 0,\ P_Z\text{-a.s.}\right\}.$$

- For separation rate $\varepsilon > 0$: $\mathcal{P}_1(\varepsilon, p, s)$, distributions P of (Z, Y) under which the ℓ_p-ECE of f is at least ε:

$$\mathcal{P}_1(\varepsilon, p, s) := \left\{P \in \mathcal{P}_{s,L,K} : \ell_p\text{-ECE}_P(f) \geq \varepsilon\right\}.$$

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- Randomly sampling new labels according to the probability predictions yields a sample from the true distribution.
- After sample splitting, we can use classical two-sample tests to check if the two samples are from the same distribution.

Experiment

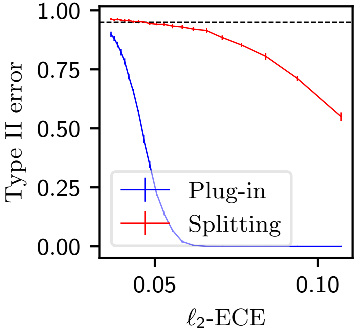

Figure: $s = 0.6$, $\rho = 100$

- Due to sample splitting, effective sample size is smaller than that of T-Cal.

Overview

Plug-in Estimator

- Recall

$$\ell_2\text{-ECE}(f)^2 = \mathbb{E}_{Z \sim P_Z}\left[\|\mathrm{reg}_f(Z) - Z]\|_2^2\right]$$

- Given a partition $\mathcal{B}_m = \{B_1, \ldots, B_{m^{K-1}}\}$ of Δ_{K-1}, with

$$\mathcal{I}_i := \{j \in \{1, \ldots, N\} : Z_j \in B_i\},$$

  the plug-in estimator for $\ell_2\text{-ECE}(f)^2$ by piecewise averaging is defined as

$$T^{\mathrm{b}}_{m,n} := \sum_{\substack{i \in [m^{K-1}] \\ |\mathcal{I}_i| \geq 1}} \frac{|\mathcal{I}_i|}{n} \left\| \frac{1}{|\mathcal{I}_i|} \sum_{j \in \mathcal{I}_i} (Y_j - Z_j) \right\|^2 . \tag{1}$$

Bias of the Plug-in Estimator

- Consider $K = 2$, $Z \sim P_Z = \text{Unif}[0,1]$, $P_0 : P_Z \times \text{Ber}(Z)$ and $P_1 : P_Z \times \text{Ber}(\text{reg}_f(Z))$ depicted below (left).

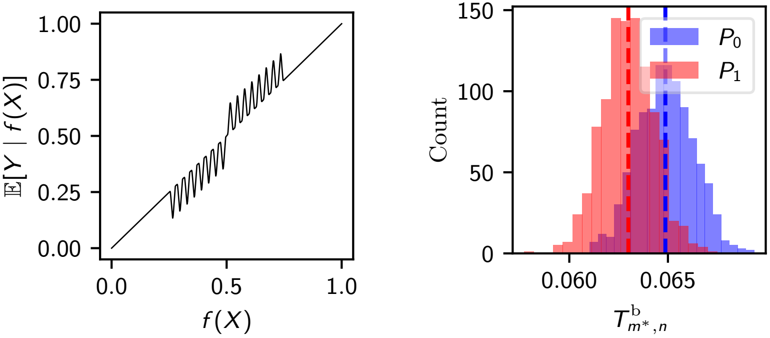

Figure: **Left:** A graph of the calibration curve $z \mapsto \text{reg}_f(z)$ under P_1. **Right:** Histograms of $T^{\mathrm{b}}_{m,n}$ and $T^{\mathrm{d}}_{m,n}$ under P_0 and P_1 are obtained from $1,000$ independent observations.

Debiasing the Plug-in Estimator

- The plug-in estimator is biased, because we are estimating both $\mathbb{E}[Y \mid Z \in B_i]$ and $\mathbb{E}[Z \mid Z \in B_i]$ using the same sample $(Z_i, Y_i), i \in \{1, \ldots, n\}$.

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- We define the *Debiased Plug-in Estimator* (DPE):

$$T^{\mathrm{d}}_{m,n} = \sum_{\substack{i \in [m^{K-1}] \\ |\mathcal{I}_i| \geq 1}} \frac{1}{n|\mathcal{I}_i|} \left[\left\| \sum_{j \in \mathcal{I}_i} (Y_j - Z_j) \right\|^2 - \sum_{j \in \mathcal{I}_i} \| Y_j - Z_j \|^2 \right].$$

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- The mean of $T^{\mathrm{d}}_{m,n}$ is not exactly ℓ_2-ECE$(f)^2$ under $P \in \mathcal{P}_1(\varepsilon, p, s)$, but debiasing makes it comparable to ℓ_2-ECE$(f)^2$.

T-Cal: Debiased Plug-in Test

- We use $T^{\mathrm{d}}_{m,n}$ as our test statistic.

$$\xi_{m,n}(\alpha) = \xi_{m,n} := \begin{cases} I\left(T^{\mathrm{d}}_{m,n} \geq \sqrt{\frac{2K}{\alpha}} m^{\frac{K-1}{2}} n^{-1}\right) & \text{if } m^{K-1} \leq n, \\ I\left(T^{\mathrm{d}}_{m,n} \geq \sqrt{\frac{2K}{\alpha}} m^{-\frac{K-1}{2}}\right) & \text{if } m^{K-1} > n. \end{cases}$$

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- One can choose critical values by bootstrapping (or, consistency resampling) in practice.

Main Theorem I

Theorem (T-Cal: Calibration test via debiased plug-in estimation)

Suppose $p \leq 2$. For $m^* = \lfloor n^{2/(4s+K-1)} \rfloor$, we have

1. **False detection rate control.** *For every P for which f is calibrated, i.e., for $P \in \mathcal{P}_0$, the probability of falsely claiming mis-calibration is at most α, i.e., $P(\xi_{m^*,n} = 1) \leq \alpha$.*

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2. **True detection rate control.** *There exists $c > 0$ depending on $(s, L, K, \nu_l, \nu_u, \alpha, \beta)$ such that the power (true positive rate) is bounded as $P(\xi_{m^*,n} = 1) \geq 1 - \beta$ for every $P \in \mathcal{P}_1(\varepsilon, p, s)$—i.e., when f is mis-calibrated with an ℓ_p-ECE of at least*

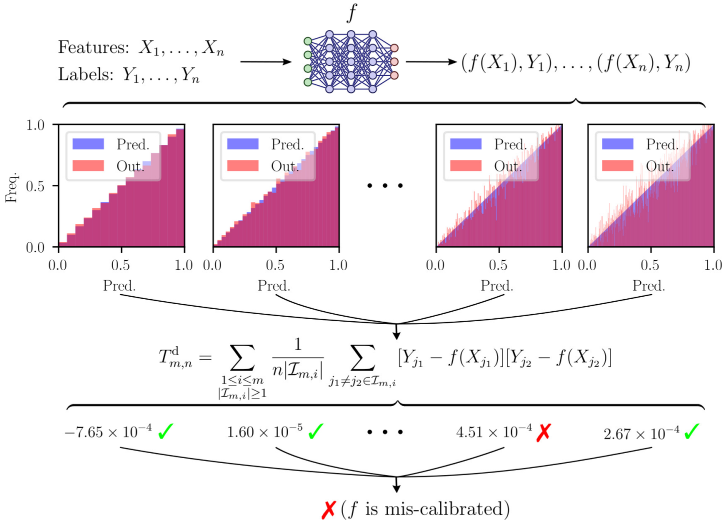
$$\varepsilon \geq cn^{-\frac{2s}{4s+K-1}}.$$

Combined with lower bounds we show, T-Cal is minimax optimal over Hölder smooth calibration curves

Adaptive T-Cal

For a number $B = \lceil \frac{2}{K-1} \log_2(n/\sqrt{\log n}) \rceil$ of tests performed, let

$$\xi_n^{\mathrm{ad}} := \max_{b \in \{1,\ldots,B\}} \xi_{2^b,n}\left(\frac{\alpha}{B}\right).$$



Main Theorem II: Adaptive T-Cal

Theorem (Adaptive T-Cal)

Suppose $p \leq 2$*. The adaptive test* ξ_n^{ad} *enjoys*

1. **False detection rate control.** *For every* P *for which* f *is calibrated, i.e., for* $P \in \mathcal{P}_0$*, the probability of falsely claiming mis-calibration is at most* α*, i.e.,* $P\left(\xi_n^{\mathsf{ad}} = 1\right) \leq \alpha$*.*

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2. **True detection rate control.** *There exists $c_{\mathrm{ad}} > 0$ depending on $(s, L, K, \nu_l, \nu_u, \alpha, \beta)$ such that the power (true positive rate) is lower bounded as $P(\xi_n^{\mathrm{ad}} = 1) \geq 1 - \beta$ for every $P \in \mathcal{P}_1(\varepsilon, p, s)$—i.e., when f is mis-calibrated with an ℓ_p-ECE of at least*

$$\varepsilon \geq c_{\mathrm{ad}}(n/\sqrt{\log n})^{-\frac{2s}{4s+K-1}}.$$

Overview

Synthetic data

- We compare T-Cal with classical calibration tests [2, 9, 4, 10]:
  - Cox's Logistic Score test
  - test based on plug-in $\widehat{\ell_1\text{-ECE}}$

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  - Cox's Logistic Score test
  - test based on plug-in $\widehat{\ell_1\text{-ECE}}$
- $H_1 : (Z, Y) \sim P_{1,m}$

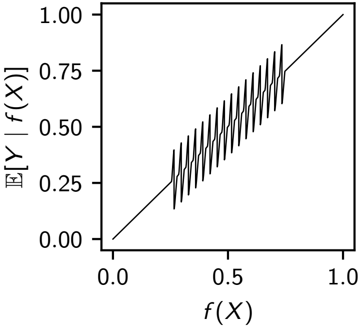

Figure: Calibration curve under $P_{1,m}$

Synthetic data results: T-Cal vs other tests

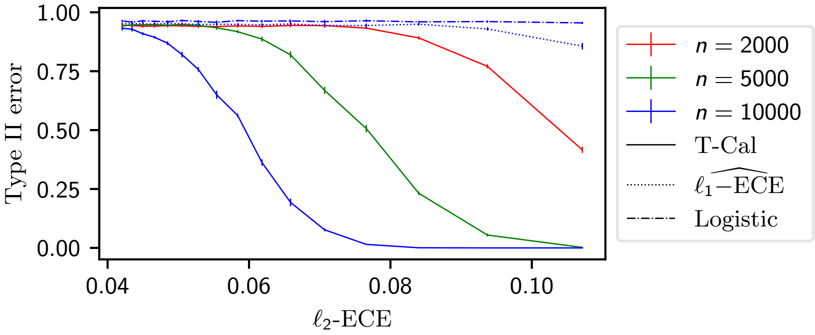

Figure: Comparison of calibration tests: T-Cal (with m^*) is more sample-efficient than other methods (with $n = 10,000$)

Synthetic data ablation: m^*, debiasing, ℓ_2 vs ℓ_1

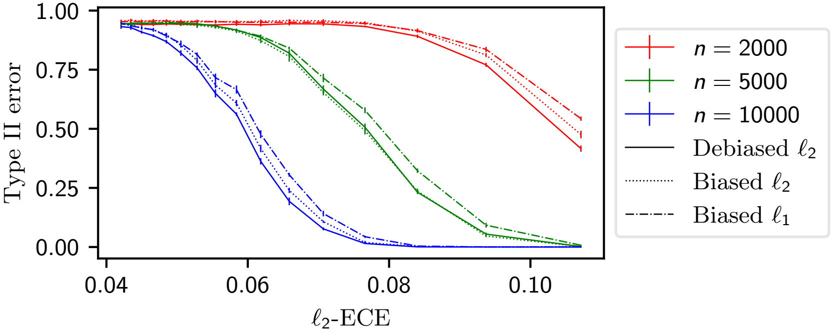

Figure: Type II error comparison for $T^{\mathrm{d}}_{m^*,n}$ (T-Cal), $T^{\mathrm{b}}_{m^*,n}$, and $T^{\ell_1}_{m^*,n}$. Using ℓ_2 is better than ℓ_1, and debiased ℓ_2 (T-Cal) is better than biased ℓ_2. Standard error bars are plotted over 10 repetitions. m^* has largest effect.

Empirical data

- We test adaptive T-Cal on various deep neural networks trained on CIFAR-10/100 and ImageNet.

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- We test adaptive T-Cal on various deep neural networks trained on CIFAR-10/100 and ImageNet.
- We test models calibrated by standard post-hoc methods (and uncalibrated ones).

Results on empirical data: CIFAR-10

	DenseNet 121		ResNet 50		VGG-19	
	$\widehat{\ell_1\text{-ECE}}$	Calibrated?	$\widehat{\ell_1\text{-ECE}}$	Calibrated?	$\widehat{\ell_1\text{-ECE}}$	Calibrated?
No Calibration	2.02%	reject	2.23%	reject	2.13%	reject
Platt Scaling	2.32%	reject	1.78%	reject	1.71%	reject
Poly. Scaling	1.71%	reject	1.29%	reject	0.90%	accept
Isot. Regression	1.16%	reject	0.62%	reject	1.13%	accept
Hist. Binning	0.97%	reject	1.12%	reject	1.28%	reject
Scal. Binning	1.94%	reject	1.21%	reject	1.67%	reject

Table 1: The values of the empirical ℓ_1-ECE (Guo et al., 2017) and the testing results, via adaptive T-Cal and multiple binomial testing, of models trained on CIFAR-10.

Figure: Results roughly align with the magnitude of the empirical ECE.

Results on empirical data: CIFAR-100

	MobileNet-v2		ResNet 56		ShuffleNet-v2	
	$\widehat{\ell_1\text{-ECE}}$	Calibrated?	$\widehat{\ell_1\text{-ECE}}$	Calibrated?	$\widehat{\ell_1\text{-ECE}}$	Calibrated?
No Calibration	11.87%	reject	15.2%	reject	9.08%	reject
Platt Scaling	1.40%	accept	1.84%	accept	1.34%	accept
Poly. Scaling	1.69%	reject	1.91%	reject	1.81%	accept
Isot. Regression	1.76%	accept	2.33%	reject	1.38%	accept
Hist. Binning	1.66%	reject	2.44%	reject	2.77%	reject
Scal. Binning	1.85%	reject	1.57%	reject	1.65%	accept

Table 2: The values of the empirical ℓ_1-ECE (Guo et al., 2017) and the testing results, via adaptive T-Cal and multiple binomial testing, of models trained on CIFAR-100.

Figure: Results roughly align with the magnitude of the empirical ECE. However, T-Cal *not* the same as ℓ_1-ECE: see ResNet-56.

Results on empirical data: CIFAR-10, reliability diagrams

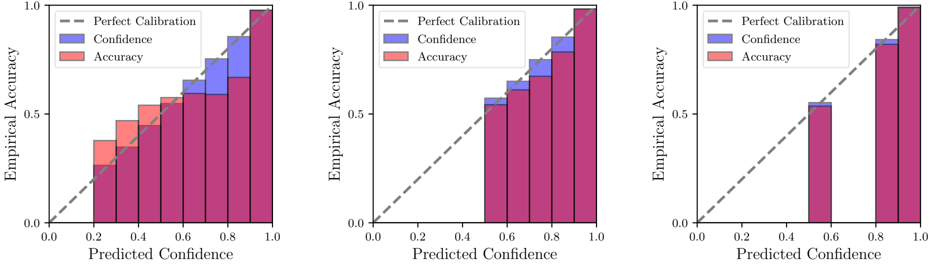

Figure: The reliability diagrams for VGG-19, trained on CIFAR-10, calibrated by Platt scaling (left - reject), polynomial scaling (middle - accept), and histogram binning (right - accept). Bins containing less than 10 data points, where the sample noise dominates, are omitted for clarity.

Results on empirical data: ImageNet

	DenseNet 161		ResNet 152		EfficientNet-b7	
	$\widehat{\ell_1\text{-ECE}}$	Calibrated?	$\widehat{\ell_1\text{-ECE}}$	Calibrated?	$\widehat{\ell_1\text{-ECE}}$	Calibrated?
No Calibration	5.67%	reject	4.99%	reject	2.82%	reject
Platt Scaling	1.58%	reject	1.41%	reject	1.90%	reject
Poly. Scaling	0.62%	accept	0.64%	accept	0.71%	accept
Isot. Regression	0.63%	reject	0.80%	reject	1.06%	reject
Hist. Binning	0.46%	reject	1.26%	reject	0.88%	reject
Scal. Binning	1.55%	reject	1.40%	reject	1.97%	reject

Table 3: The values of the empirical ℓ_1-ECE (Guo et al., 2017) and the testing results, via adaptive T-Cal and multiple binomial testing, of models trained on ImageNet.

Overview

Impossibility for continuous mis-calibration curves

- If the mis-calibration curve can oscillate with arbitrarily high frequency, mis-calibration cannot be detected from a finite sample. (Caution when using complex models!)

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- If the mis-calibration curve can oscillate with arbitrarily high frequency, mis-calibration cannot be detected from a finite sample. (Caution when using complex models!)
- Define minimax type II error for distributions in the alternative with continuous mis-calibration curves

$$R_n^{\text{cont}}(\varepsilon, p) := \inf_{\xi \in \Phi_n(\alpha)} \sup_{P \in \mathcal{P}_1^{\text{cont}}(\varepsilon, p)} P(\xi = 0).$$

Proposition

Let $\varepsilon_0 = 0.1$. For any level $\alpha \in (0, 1)$, the minimax type II error $R_n^{\text{cont}}(\varepsilon_0, p)$ for testing the null hypothesis of calibration at level α against the hypothesis $P \in \mathcal{P}_1^{\text{cont}}(\varepsilon_0, p)$ of continuous mis-calibration curves satisfies

$$R_n^{\text{cont}}(\varepsilon_0, p) \geq 1 - \alpha$$

for all n.

Hölder continuous calibration curves

- We consider detecting mis-calibration when the mis-calibration curves are Hölder continuous; as usual in nonparametric statistics [5, 8, 3, 6].

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- Rich class of mis-calibration curves, including non-smooth ones.

Lower bound for Hölder continuous mis-calibration curve

- Test the calibration of the K-class probability predictor f assuming (s, L)-Hölder continuity of mis-calibration curves at a level $\alpha \in (0, 1)$.
- Minimax type II error

$$R_n(\varepsilon, p, s) := \inf_{\xi \in \Phi_n(\alpha)} \sup_{P \in \mathcal{P}_1(\varepsilon, p, s)} P(\xi = 0).$$

- Minimum separation needed for a minimax type II error of at most β

$$\varepsilon_n(p, s) = \inf\{\varepsilon' : R_n(\varepsilon', p, s) \leq \beta\}.$$

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Theorem

There exists $c_{\text{lower}} > 0$ depending only on $(p, s, L, K, \alpha, \beta)$ such that, for any $p > 0$, the minimum ℓ_p-ECE of f, i.e. $\varepsilon_n(p, s)$, required to have a test with a false positive rate (type I error) at most α and with a true positive rate (power) at least $1 - \beta$ satisfies

$$\varepsilon_n(p, s) \geq c_{\text{lower}} n^{-\frac{2s}{4s+K-1}}$$

for all n.

Context, continued

- Non-parametric rate $n^{-\frac{2s}{4s+K-1}}$ slower than parametric $n^{-1/2}$ rate. Slower as the number of classes K grows.

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- What one expects based on nonparametric two-sample goodness-of-fit testing for densities on Δ_{K-1} [6].
- T-Cal is minimax optimal.
- Evaluating multi-class model calibration on a small dataset can be challenging.

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- Uncertainty quantification important for ML. Calibration is a key problem with rich history.
  1. **The need for statistical significance to claim calibration.**
  2. **Potential suboptimality of popular approaches.**
- T-Cal: adaptive test for calibration of ML models; supported by empirical & theoretical results.
  - Available at `https://github.com/dh7401/Calibration-Test`

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$$\mathcal{V}_k := \left\{ Z_i : [Y_i]_k = 1, 1 \le i \le \left\lfloor \frac{n}{2} \right\rfloor \right\},$$

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- $\mathcal{V}_k$ and $\mathcal{W}_k$ have densities

$$\pi_k^{\mathcal{V}}(\mathrm{z}) := \frac{[\mathrm{reg}_f(\mathrm{z})]_k}{\int_{\Delta_{K-1}} [\mathrm{reg}_f(\mathrm{z})]_k dP_Z(\mathrm{z})} = \frac{[\mathrm{reg}_f(\mathrm{z})]_k}{\mathbb{E}[Y]_k},$$

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with respect to P_Z.

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\begin{aligned}
T_{1,k} &= \frac{1}{n}\sum_{i=1}^{n}[Y_i - Z_i]_k, \\
T_{2,k} &= \frac{1}{n}\sum_{i=1}^{n}[Z_i]_k[Y_i - Z_i]_k, \\
b_k &= I\left(|T_{1,k}| \geq \sqrt{\frac{3K}{\alpha n}}\right) \vee I\left(|T_{2,k}| \geq \sqrt{\frac{3K}{\alpha n}}\right) \vee \mathtt{TS}_{\frac{\alpha}{3K},\frac{\beta}{2}}(\mathcal{V}_k, \mathcal{W}_k).
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- Reject H_0 if $\max\{b_1, \dots, b_K\} = 1$.

Main Result: Known smoothness

Theorem (Optimal calibration test via sample splitting)

Suppose $p \leq 2$ and let ξ_n^{split} be the test described in the previous slide. Assume the Hölder smoothness parameter s is known. We have

1. **False detection rate control.** *For every P for which f is calibrated, i.e., for $P \in \mathcal{P}_0$, the probability of falsely claiming mis-calibration is at most α, i.e., $P(\xi_n^{\text{split}} = 1) \leq \alpha$.*

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$$\varepsilon \ge c_{\text{split}} n^{-\frac{2s}{4s+K-1}}.$$

Main Result: Adapting to smoothness

- Consider an adaptive two-sample goodness-of-fit test $\mathtt{TS}^{\mathrm{ad}}_{\alpha,\beta}$.

Corollary (Adaptive test via sample splitting)

Suppose $p \le 2$ and let $\xi_n^{\text{ad-s}}$ be the test described abvoe with $\mathtt{TS}$ *replaced by an adaptive two-sample test* $\mathtt{TS}^{\mathrm{ad}}$. *We have*

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