Counterfactually Comparing Abstaining Classifiers

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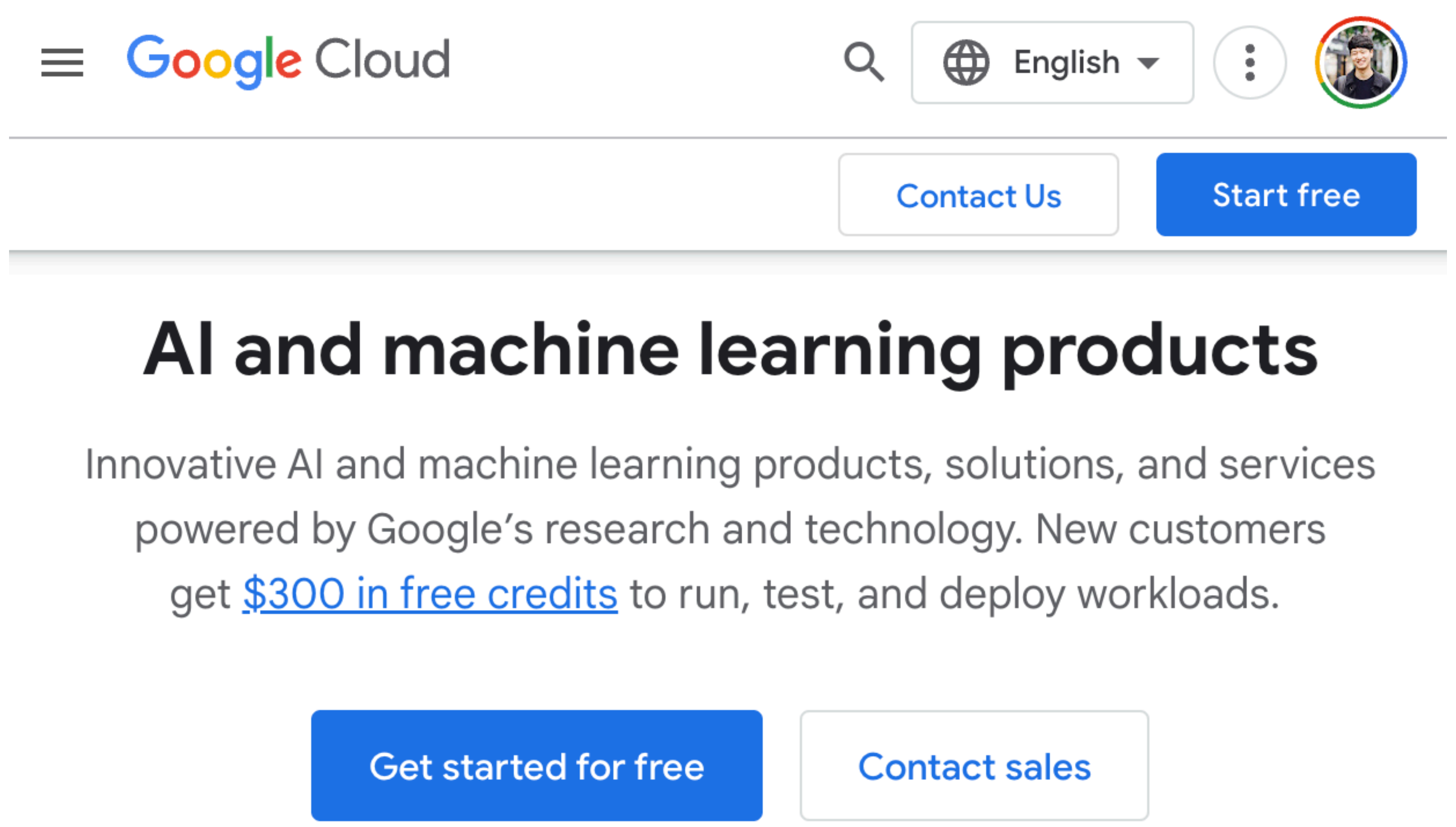
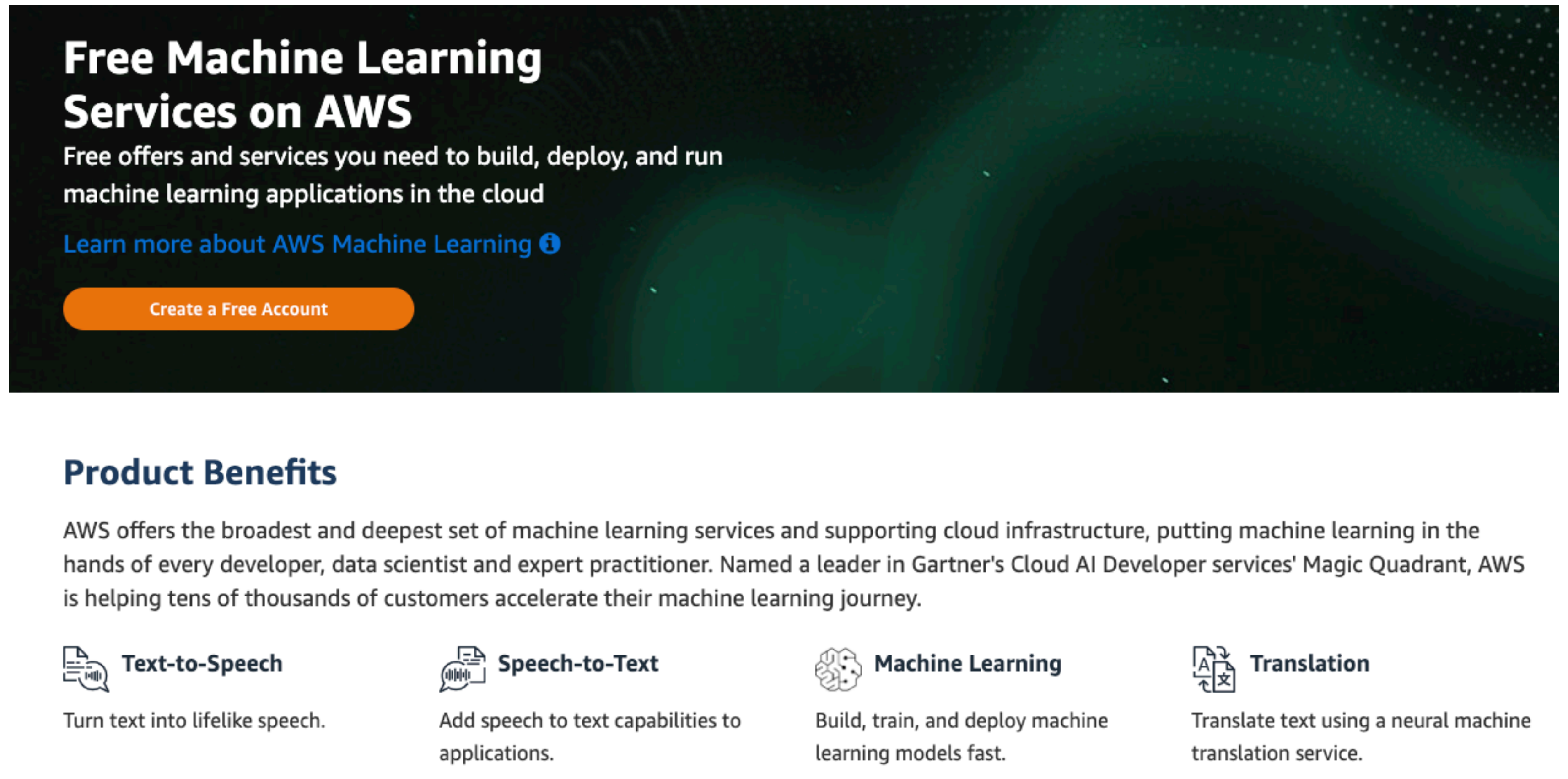
Motivation: Evaluating Free-Trial ML Services

- Suppose that we want to evaluate **black-box** ML prediction services for image classification.

- During the **free trial**, each service deploys an abstaining classifier, such that it only gives predictions on certain inputs and abstain on others.

- **The full (paid) versions do not abstain.** We want to compare the performance of the full versions.





Key Takeaway & Main Question

To the evaluator, abstentions are just **missing** predictions!

How do we compare black-box abstaining classifiers

while accounting for their missing predictions?

Problem Setup

Chow (1957); El-Yaniv & Wiener (2010)

Definition. An **abstaining classifier** is a pair of functions (f, π), where

- $f : \mathscr{X} \to \mathscr{P}(\mathscr{Y})$ is the **base classifier**, which outputs a (probabilistic) prediction; and
- $\pi : \mathscr{X} \to [0, 1]$ is the **abstention mechanism**, which outputs the probability of abstention.

Evaluating a black-box abstaining classifier (f, π).

1. Classifier receives an input X.
2. Classifier decides whether or not it will abstain: $R \mid X \sim \text{Ber}(\pi(X))$.
   - If $R = 0$, then Evaluator observes the prediction & score: $S = s(f(X), Y)$.
   - If $R = 1$ ("rejection"), then Evaluator does NOT see its prediction or score **(S is missing)**.

The 3-Step Approach To Nonparametric Causal Inference

Target Definition → **Identification** → **Estimation**

Target Definition

$$\psi \stackrel{\text{def}}{=} \mathbb{E}[S]$$

("Counterfactual Score")

Nuisance Functions (Learnable):

Abstention Mechanism

$$\pi(X) \stackrel{\text{def}}{=} \mathbb{P}(R = 1 \mid X)$$

Selective Score Predictor

$$\mu_0(X) \stackrel{\text{def}}{=} \mathbb{E}[S \mid R = 0, X]$$

Identification

$$\psi = \mathbb{E}[\mu_0(X)]$$

Conditions

1. **Missing At Random:** $S \perp\!\!\!\perp R \mid X$ — Independent Evaluation Set
2. **Positivity:** $\pi(X) \leq 1 - \epsilon$ (for some $\epsilon > 0$) — Stochastic Abstentions

Estimation

$$\sqrt{n}\left(\hat{\psi}_{\text{dr}} - \psi\right) \rightsquigarrow \mathcal{N}\left(0, \text{Var}_{\mathbb{P}}[\text{IF}]\right)$$

Conditions

1. **Double Robustness:** $\|\hat{\pi} - \pi\|_{L^2} \|\hat{\mu}_0 - \mu_0\|_{L^2} = o_{\mathbb{P}}(1/\sqrt{n})$ — Flexible Nuisance Learners (NN, RF, ...)
2. **IF Consistency:** $\|\hat{\text{IF}} - \text{IF}\| = o_{\mathbb{P}}(1)$

cf. Rubin (1974); Robins et al. (1994); many others.

Other names: augmented IPW (Robins et al., 1994);
targeted MLE (van der Laan & Rubin, 2006);
double ML (Chernozhukov et al., 2018)

The Doubly Robust Estimator $\hat{\psi}_{\mathrm{dr}}$

Given an *i.i.d.* data of potentially missing predictions, $\{(X_i, R_i, (1 - R_i)S_i)\}_{i=1}^{n} \sim \mathbb{P}$, the **doubly robust (DR) estimator for ψ** is defined as:

$$\hat{\psi}_{\mathrm{dr}} = \frac{1}{n} \sum_{i=1}^{n} \left[\hat{\mu}_0(X_i) + \frac{1 - R_i}{1 - \hat{\pi}(X_i)} \left(S_i - \hat{\mu}_0(X_i) \right) \right].$$

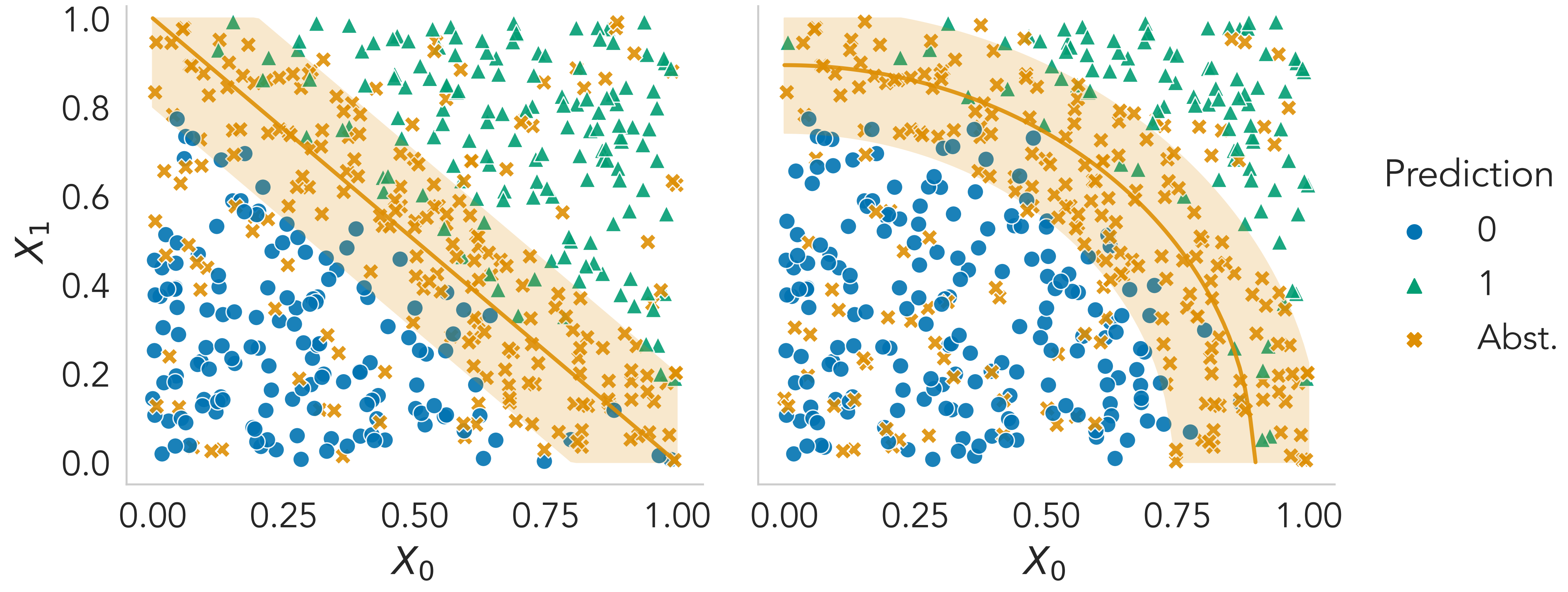
The summand is the **influence function** for $\mathbb{E}[\mu_0(X)]$ (a first-order bias correction).

For comparison, we can simply take the difference between the two classifiers ($\hat{\psi}^{A}_{\mathrm{dr}} - \hat{\psi}^{B}_{\mathrm{dr}}$).

*The nuisance functions, $\hat{\mu}_0$ and $\hat{\pi}$, are estimated via **cross-fitting** (K-fold sample splitting).

Simulated Experiment: CI Miscoverage & Width

A: linear classifier with the <u>*optimal*</u> decision boundary. **B:** <u>*biased*</u> classifier with a curved boundary.



Two abstaining classifiers, depicted using their decision boundary (orange), predictions (●/▲), and abstentions (x).

$\hat{\pi}$ / $\hat{\mu}_0$	*95% CI's*	Plug-in	IPW	DR
Random Forest	*Miscoverage*	0.64	0.14	**0.05**
	Width	*0.02*	*0.13*	*0.07*
Super Learner	*Miscoverage*	0.91	**0.03**	**0.05**
	Width	*0.01*	*0.12*	*0.06*

CI Miscoverage: rate of the 95% CI not covering the true Δ^{AB}, based on *accuracy*.
(**Blue**: valid miscoverage.)
Width: upper minus lower confidence bound.
Both averaged over 1,000 repeated simulations.

DR CI achieves the correct miscoverage rate **(small bias)**, and its width is half the width of the IPW CI **(small variance)**.

Real Data Experiment: Comparing VGG-16 Classifiers on CIFAR-100

- **Setup:** We compare abstaining classifiers based off of a pre-trained VGG-16 deep convolutional neural network* for the CIFAR-100 dataset. Evaluation set size is 5,000.
- Nuisance functions $(\hat{\pi}^{\mathrm{A}}, \hat{\mu}_0^{\mathrm{A}}, \hat{\pi}^{\mathrm{B}}, \hat{\mu}_0^{\mathrm{B}})$ are learned on top of the pre-trained VGG-16 network, but they each use a different output layer (learned via cross-fitting).

Scenarios	Base Classifier	Abstention Rule	$\bar{\Delta}^{\mathrm{AB}}$	95% DR CI	Reject H_0?
I	Same	Different	0.000	(-0.005, 0.018)	No
II	Same	Different	0.000	(-0.014, 0.008)	No
III	Different	Same	−0.029	(-0.051, -0.028)	Yes

Comparing VGG-16-Based Abstaining Classifiers on CIFAR-100 (n=5,000) using the Brier score.
Estimation target: $\Delta^{\mathrm{AB}} := \psi^{\mathrm{A}} - \psi^{\mathrm{B}}$; null hypothesis $\mathrm{H}_0 : \Delta^{\mathrm{AB}} = 0$.

*reproduced version from https://github.com/chenyaofo/pytorch-cifar-models.

Summary of Contributions

- We propose the ***counterfactual score***, a novel evaluation metric for black-box abstaining classifiers that assess the expected score had the classifier not been allowed to abstain.
- The score and its framework reveals an **underexplored connection** between abstaining classifiers, black-box evaluation, and missing data / causal inference.
- We formalize the **identifying assumptions (MAR and positivity)** for the score and give examples of settings in which they can be justified.
- We develop **nonparametrically efficient** estimators for the counterfactual score (difference), and empirically show their validity & efficiency on simulated/real datasets.

Thank You

Paper: https://arxiv.org/abs/2305.10564
Code: https://github.com/yjchoe/ComparingAbstainingClassifiers
NeurIPS Link: https://neurips.cc/virtual/2023/poster/72515
YJ's Webpage (for links to slides & poster): https://yjchoe.github.io/

Poster Session: **Tuesday Evening** (5:15-7:15pm CT on December 12th) / Poster #: **1618**