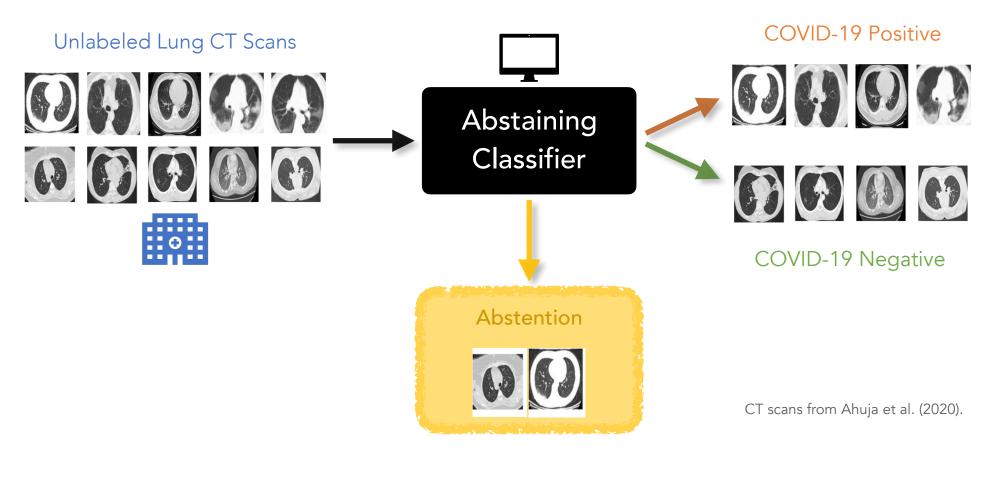
Counterfactually Comparing Abstaining Classifiers

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Abstaining classifiers

Abstaining classifiers (Chow, 1957) have the option to withhold their predictions on inputs that they are uncertain about. They are used in safety-critical applications, such as medical imaging.



How can we evaluate and compare black-box abstaining classifiers?

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- Suppose we want to evaluate and compare black-box ML prediction services for an image classification task.
- During the free trial, each service deploys an abstaining classifier. Each classifier utilizes its own (unknown) abstention mechanism.
- Once you pay for each service, it will use a non-abstaining classifier. How can we compare the expected accuracies without accessing them?

To the evaluator, abstentions are just missing predictions!

The counterfactual question

How would we compare black-box abstaining classifiers, had they not been allowed to abstain?

We propose a **black-box** evaluation framework for abstaining classifiers by leveraging tools from *missing data analysis* (Rubin, 1976) and *nonparametric causal inference* (e.g., Robins et al., 1994).



The counterfactual approach

An abstaining classifier (AC) is a pair of functions (f, π) , where

- $f: \mathcal{X} \to \mathcal{Y}$ is the base classifier (f(X): prediction);
- $\pi : \mathscr{X} \to [0, 1]$ is the abstention mechanism ($\pi(X)$: prob. of abstention).

Protocol (Evaluating a black-box abstaining classifier).

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

Step 1: Defining the counterfactual score

The counterfactual score ψ of an AC (f, π) is its expected score:

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

For comparison, estimate $\Delta = \psi^{A} - \psi^{B} = \mathbb{E}[S^{A} - S^{B}]$.

Step 2: Identification

Under identifying conditions,

 $\psi = \mathbb{E}[\mu_0(X)], \text{ where } \mu_0(X) = \mathbb{E}[S \mid X, R = 0].$

What are the identifying conditions?

- **1. Missing at random (MAR):** $S \perp R \mid X$.
 - Satisfied as long as the evaluation set is *independent* of training set.
- **2.** Positivity: There exists $\varepsilon > 0$ such that $\pi(X) \le 1 \varepsilon$.
 - Satisfied as long as the classifier does not *deterministically* abstain on an input region. (Otherwise it's impossible to estimate the score!)

Step 3: Doubly robust estimation

Now, define the doubly robust (DR) estimator $\hat{\psi}_{dr}$:

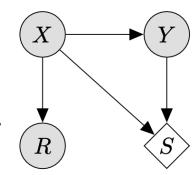
$$\hat{\psi}_{dr} = \frac{1}{n} \sum_{i=1}^{n} \left[\hat{\mu}_{0}(X_{i}) + \frac{1 - R_{i}}{1 - \hat{\pi}(X_{i})} \left(S_{i} - \hat{\mu}_{0}(X_{i}) \right) \right],$$

where $\hat{\mu}_0$ and $\hat{\pi}$ are nuisance function estimators (e.g., ensemble methods).

<u>Theorem (Informal)</u>. With sufficiently flexible nuisance function estimators $\hat{\mu}_0$ and $\hat{\pi}$, the DR estimator is **asymptotically normal and efficient for** ψ :

$$\sqrt{\mathsf{n}}\left(\hat{\psi}_{\mathsf{dr}} - \psi\right) \leadsto \mathscr{N}\left(\mathsf{0}, \mathsf{Var}_{\mathbb{P}}(\mathsf{IF})\right).$$

The nuisance functions are estimated via cross-fitting (Robins et al., 2008).



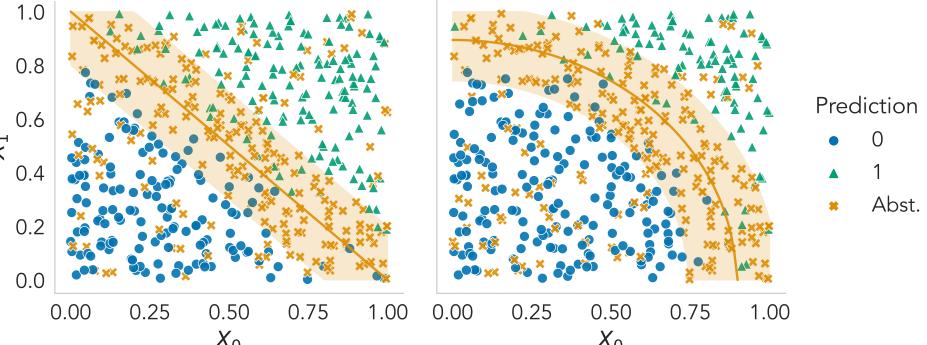


Experiments

Simulated data: Comparing abstaining binary classifiers (MAR)

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 (\bullet/\blacktriangle), and abstentions (x).

Nuisance fn.	95% Cl'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

Miscoverage and width of the 95% CI for estimating Δ^{AB} , based on *accuracy*. Baselines: plug-in & IPW. N=2,000; averaged over 1,000 repeated simulations.

The doubly robust CI achieves the correct miscoverage rate while having a small width (i.e., it is efficient).

Real data: comparing abstaining CNNs for image classification

Base clf.	Abstention	Δ	Reject null?	95% CI
Same	Different	0.000	Νο	(-0.014, 0.008)
Different	Same	-0.029	Yes	(-0.051, -0.028)

Hypothesis tests and 95% CIs for comparing abstaining classifiers built using pre-trained VGG-16 networks on CIFAR-100 dataset (N=5,000). Null: $\Delta = 0$.

The theory is applicable to testing or estimating the counterfactual score difference between nonparametric predictors.

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