Counterfactually Comparing Abstaining Classifiers

Yo Joong Choe, Aditya Gangrade, and Aaditya Ramdas 37th Conference on Neural Information Processing Systems (NeurIPS 2023)



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Abstaining Classifiers Chow (1957) a.k.a. Selective Classifiers; Classifiers with a Reject Option

Unlabeled Lung CT Scans





Sample lung CT scans of (non-)COVID patients from Ahuja et al. (2020). 2



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.

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Key Takeaway & Main Question

To the evaluator, abstentions are just missing predictions!

while accounting for their missing predictions?

How do we compare black-box abstaining classifiers

Problem Setup

<u>Definition</u>. An abstaining classifier is a pair of functions (f, π) , where

- $f: \mathcal{X} \to \mathscr{P}(\mathcal{Y})$ 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

- 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 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).

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



Illustration: Evaluating a Black-Box Abstaining Classifier



*Base classifier & abstention mechanism may be conjoined (e.g., via shared feature layers).

Yellow: only observed when R = 0.





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

Target Definition

Target Definition

Identification

Estimation

Our Target: The Counterfactual Score

Definition (Counterfactual Score): Given an abstaining classifier, we define the **counterfactual score** ψ as

where S = s(f(X), Y) for some scoring function s (e.g., accuracy & Brier score). Expectation \mathbb{E} is taken over (X, R, S). No conditioning on non-abstentions (R = 0).

Why the counterfactual score?

- There exist efficient estimators that do not require parametric modeling assumptions.

 $\psi = \mathbb{E}[S],$

NOTE: S is missing when R = 1.

Measures how each classifier would have performed, had it not been allowed to abstain.



The Popular Metric Does NOT Account for Missing Predictions

It is common to evaluate abstaining classifier using selective score & coverage (a two-dimensional metric):

- Selective score = expected score only on selections (non-abstentions) = $\mathbb{E}[S \mid R = 0]$.
- **Coverage** = expected rate of non-abstentions = $\mathbb{P}(\mathbb{R} = 0)$.

- Selective score + coverage do NOT capture the classifier's performance adequately,
 - particularly when the missing predictions matter.

For Comparison: The Counterfactual Score Difference

we define their counterfactual score difference Δ as



where $S^A := s(f^A(X), Y)$ and $S^B := s(f^B(X), Y)$ for some scoring function s. Expectation \mathbb{E} is taken over (X, R^A, S^A, R^B, S^B) . No conditioning on non-abstentions.

<u>Remark</u>: The two classifiers can operate under their **separate abstention mechanisms**.

Definition (Counterfactual Score Difference): given two abstaining classifiers, A & B,

 $\Delta := \mathbb{E}[\mathsf{S}^{\mathsf{A}} - \mathsf{S}^{\mathsf{B}}],$



Classifiers Can Use Separate Abstention Mechanisms

Counterfactual Score Difference

$$\Delta = \mathbb{E}[\mathsf{S}^{\mathsf{A}} - \mathsf{S}^{\mathsf{B}}]$$



may observe both, either, or neither

Average Treatment Effect $\mathsf{ATE} = \mathbb{E}[\mathsf{Y}^1 - \mathsf{Y}^0]$



observe one or the other



Identification

Target Definition

Identification

Estimation

Identifying Condition #1: Missing-at-Random

The missing-at-random (MAR) condition says that, given the input X, the decision to abstain R is independent of the base classifier's score S = s(f(X), Y):

S ⊥ R | X.

- MAR is satisfied as long as the evaluation data is independent from the classifier (Ppn. 4.1).
- Typically, predictions are **NOT** missing **completely** at random (MCAR), i.e., SHR.

(a.k.a. ignorability & no unmeasured confounding)



Conditioned on X, S and R are d-separated.

Diamond <S> means partially observed. (cf. missingness graphs by Mohan et al., 2013)

Can the MAR Condition Ever Be Violated?

- The MAR condition is met as long as $(X, Y) \perp \mathcal{D}_{train}$ (Ppn. 4.1), i.e., the classifier's training data is *independent* from the test data.
 - This is expected in a typical setup for evaluating learning algorithms.
 - If a classifier already saw the test data, then it would surely do better.
- Unfortunately, in a purely black-box setting, the evaluator may not know what training data was used by the classifier.
 - E.g., large ML models pre-trained on publicly available datasets.
- **Practical suggestions for preventing/addressing MAR violations:**
 - Use a test set that is not publicly available (e.g., patient data).
 - Conduct sensitivity analysis, e.g., under a contamination model (Bonvini & Kennedy, 2022).



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Identifying Condition #2: Positivity

The positivity condition for this problem requires that each abstaining classifier cannot deterministically abstain (on any meaningful input region):

 $\exists \epsilon > 0 : \quad \pi(\mathsf{X}) = \mathbb{P}(\mathsf{R} = 1 \mid \mathsf{X}) \le 1 - \epsilon.$

This is a **necessary** condition:

there is no way of knowing what it would have done in that region.

• If a classifier deterministically abstains on some nontrivial part of the input space, then

How Can We Address the Positivity Condition?

- Positivity violations can affect the validity and efficiency of the estimator.
 - Yet, in practice, classifiers may abstain deterministically on certain inputs.
- Argument 1: unidentifiability & a need for a policy-level approach.
 - If a governing body seeks to audit commercial softwares for safety-critical tasks, then they must **require** vendors to match a level of positivity.
- Argument 2: stochastic abstentions can improve performances.
 - Kalai & Kanade (2021) showed that stochastic abstentions can improve out-of-distribution (OOD) performance of abstaining classifiers.
 - Schreuder & Chzhen (2021) derived a stochastically abstaining classifier that achieves good performance subject to a fairness constraint.



For $\epsilon < 0.2$,

the miscoverage rate of a 95% CI rises above the intended level.



Identification

score as an expectation over observables:

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

where μ_0 is the score regression function: μ_0

In other words, the target parameter can now be estimated with observed data.

The rest of the problem is purely that of *functional estimation* (nothing causal).

Proposition. Under the MAR and positivity conditions, we can identify the counterfactual

$$\mathbf{x}_{0}(\mathbf{x}) = \mathbb{E}[\mathbf{S} \mid \mathbf{R} = \mathbf{0}, \mathbf{X} = \mathbf{x}].$$

One-Line Proof of Identification

score as following:

where μ_0 is the score regression function: μ_0

One-line proof using standard arguments: μ_0 is well-defined by positivity; then,

Proposition. Under the MAR and positivity conditions, we can identify the counterfactual

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

$$_{0}(\mathbf{x}) = \mathbb{E}[\mathbf{S} \mid \mathbf{R} = \mathbf{0}, \mathbf{X} = \mathbf{x}].$$

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

Identification for Δ^{AB}

Under the identifying assumptions, we have that:

 $\Delta^{\mathsf{A}\mathsf{B}} = \mathbb{E}[\mathsf{S}^\mathsf{A} - \mathsf{S}^\mathsf{B}]$

where

$$\mu_0^{\mathsf{A}}(\mathsf{x}) = \mathbb{E}[\mathsf{S}^{\mathsf{A}} \mid \mathsf{R}^{\mathsf{A}} = \mathsf{0}, \mathsf{X} = \mathsf{x}]$$

As before, the target parameter can now be estimated with observed data! The rest of the problem is purely that of function estimation (and not causal).



$$B^{B}] = \mathbb{E}[\mu_{0}^{A}(X) - \mu_{0}^{B}(X)],$$

and
$$\mu_0^{B}(x) = \mathbb{E}[S^{B} | R^{B} = 0, X = x].$$

Estimation

Target Definition

Identification

Estimation

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

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:

 $\hat{\psi}_{dr} = \frac{1}{n} \sum_{i=1}^{n} \left| \hat{\mu}_0(\mathbf{X}_i) + \mathbf{y}_0(\mathbf{X}_i) \right|^2$

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 ($\hat{\psi}_{dr}^{A} - \hat{\psi}_{dr}^{B}$).

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

$$+ \frac{1 - R_i}{1 - \hat{\pi}(X_i)} \left(S_i - \hat{\mu}_0(X_i) \right) \right].$$

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

DR Estimator is Asymptotically Normal & Efficient

hold & that the nuisance functions are estimated at a parametric rate in product:

$$\|\hat{\pi} - \pi\|_{L^2(\mathbb{P})} \|\hat{\mu}_0 - \mu_0\|_{L^2(\mathbb{P})} = o_{\mathbb{P}}(1/\sqrt{n}).$$

variance matches the nonparametric (and locally minimax) efficiency bound:

$$\sqrt{n}\left(\hat{\psi}_{dr}-\psi\right)$$

An asymptotic CI for ψ can be constructed using the empirical estimate of Var_P[IF].

<u>Theorem (DR estimation of the counterfactual score)</u>. Assume the identifying conditions

Then, assuming $\|\hat{IF} - IF\|_{L_2(\mathbb{P})} = o_{\mathbb{P}}(1)$, the DR estimator is asymptotically normal, and its

$$\xrightarrow{\mathsf{d}} \mathscr{N}\left(\mathsf{0}, \mathsf{Var}_{\mathbb{P}}[\mathsf{IF}]\right).$$



Understanding Double Robustness

The DR assumption says that the nuisance functions are estimated at a parametric rate in product:

 $\|\hat{\pi} - \pi\|_{L^{2}(\mathbb{P})}\|\hat{\mu}_{0} - \hat{\mu}_{0}\|$

In particular,

- such that the product of their rates of convergence is $o_{\mathbb{P}}(1/\sqrt{n})$.
 - models. (In practice, random forests & deep neural nets can also work.)

$$-\mu_0\|_{\mathsf{L}^2(\mathbb{P})} = \mathsf{o}_{\mathbb{P}}(1/\sqrt{\mathsf{n}}).$$

Both nuisance functions can be learned at a nonparametric rate, say, $o_{\mathbb{P}}(n^{-1/4})$,

• Allows complex nuisance learners, such as the super learner (stacking) and additive



Learning the Nuisance Functions via Cross-Fitting

Computing IF requires learning the **nuisance functions** π and μ_0 from data:

$$\hat{\pi}(\mathbf{x}) = \hat{\mathbb{P}}(\mathsf{R} = 1 \mid \mathsf{X} = \mathbf{x})$$

Cross-fitting (Robins et al., 2008) allows us to learn them without losing sample efficiency.



x); $\hat{\mu}_{0}(x) = \hat{\mathbb{E}}[S | R = 0, X = x].$

25 cf. Robins et al. (2008); Zheng & van der Laan (2011); Chernozhukov et al. (2018)



DR Estimator for the Counterfactual Score Difference

hold & that the nuisance functions are estimated at a parametric rate in product:

$$\|\hat{\pi}^{\mathsf{A}} - \pi^{\mathsf{A}}\|_{\mathsf{L}^{2}(\mathbb{P})} \|\hat{\mu}_{0}^{\mathsf{A}} - \mu_{0}^{\mathsf{A}}\|_{\mathsf{L}^{2}(\mathbb{P})} + \|\hat{\pi}^{\mathsf{B}} - \pi^{\mathsf{B}}\|_{\mathsf{L}^{2}(\mathbb{P})} \|\hat{\mu}_{0}^{\mathsf{B}} - \mu_{0}^{\mathsf{B}}\|_{\mathsf{L}^{2}(\mathbb{P})} = \mathsf{o}_{\mathbb{P}}(1/\sqrt{\mathsf{n}}).$$

Let $IF^{AB} = IF^{A} - IF^{B}$. Assuming $\|IF^{AB} - IF^{AB}\| = o_{\mathbb{P}}(1)$, the DR estimator is asymptotically normal, and its variance matches the nonparametric (and locally minimax) efficiency bound:

$$\sqrt{n} \left(\hat{\Delta}_{dr}^{AB} - \Delta^{AB} \right) \stackrel{d}{\longrightarrow} \mathcal{N} \left(0, \mathsf{Var}_{\mathbb{P}}[\mathsf{IF}^{AB}] \right)$$

An asymptotic CI for Δ^{AB} , or a hypothesis test for $H_0: \psi^A = \psi^B$, can be constructed.

<u>Theorem (DR estimation of the CF score difference)</u>. Assume the identifying conditions

cf. Robins et al. (1994); Bang & Robins (2005); many others later.



How Can We Address the Positivity Condition?

- Positivity violations can affect the validity and efficiency of the estimator.
 - Yet, in practice, classifiers may abstain deterministically on certain inputs.
- Argument 1: unidentifiability & a need for a policy-level approach.
 - If a governing body seeks to audit commercial softwares for safety-critical tasks, then they must **require** vendors to match a level of positivity.
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For $\epsilon < 0.2$,

the miscoverage rate of a 95% CI rises above the intended level.



Experiments

Simulated Experiment: Cl Miscoverage & Width

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



Two abstaining classifiers, depicted using their decision boundary (orange), predictions (\bullet/\blacktriangle), and abstentions (x).

$\hat{\pi}$ / $\hat{\mu_0}$	95% Cl's	Plug-in	IPW	D
Random Forest	Miscoverage	0.64	0.14	0.0
	Width	0.02	0.13	0.0
Super Learner	Miscoverage	0.91	0.03	0.0
	Width	0.01	0.12	0.0

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).



Simulated Experiment: Power Analysis

<u>Setup</u>: score difference (Δ^{AB}) grows larger as the



Two abstaining classifiers, depicted using their decision boundary (orange), predictions (•/ \blacktriangle), and abstentions (x). Δ^{AB} =0.1.



 Δ^{AB} increases as B shifts farther away from A.

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

- but they each use a different output layer (learned via cross-fitting).

Scenarios	Base Classifier	Abstention Rule	$ar{\Delta}^{AB}$	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: $\Delta^{AB} := \psi^A - \psi^B$; null hypothesis $H_0 : \Delta^{AB} = 0$.

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 ($\hat{\pi}^A, \hat{\mu}_0^A, \hat{\pi}^B, \hat{\mu}_0^B$) are learned on top of the pre-trained VGG-16 network,



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

Appendix

How Should We Compare Black-Box Abstaining Classifiers?





Summary of Problem Formulations & Approaches

Table 1: Problem formulation for the counterfactual evaluation of black-box abstaining classifiers. The proposed approaches are applicable to settings where the evaluator has no access to the underlying abstention mechanisms or base predictors, and they do not rely on parametric modeling assumptions.

	Evaluation	Comparison	
Classifier(s) Target	(f, π) $\psi = \mathbb{E}[S]$		
Identification	MAR & positivity		
Estimation	Doubly robust CI		
Optimality	Nonparametrically efficient		



Example #2: Secondary Diagnosis

Unlabeled Lung CT Scans



Human radiologists may still make mistakes or possess cognitive biases (Busby et al., 2018).



Black-Box Abstaining Classifier



COVID-19 Positive



COVID-19 Negative







Abstention (Rejection)



Positive Negative (maybe) (maybe)







Example #3: Self-Driving Cars

Example (Alert the Driver): Let's say a semi-autonomous car deploys an abstaining image classifier that aids its driving decisions.

When it abstains, the car alerts the driver to take back the control. But...

- Unfortunately, NHSTA* reports that Tesla Autopilot can alert the driver during the very last seconds before a crash.
- Sometimes, the driver is just asleep or inattentive**. We'd still want to avoid accidents.

Can we evaluate the abstaining classifier while accounting for its performance even on its abstentions?



"Tesla Driver Caught On Camera Apparently Asleep At The Wheel" - NBC Nightly News (Sep 9, 2019)

*NHSTA: National Highway Traffic Safety Administration (U.S.) **Research shows that the lack of active involvement correlates with tardy responses to takeover requests (Vogelpohl et al., 2019).



Abstentions as Missing Predictions

These examples illustrate cases where abstentions are really missing predictions that we'd like to know.

- The free-trial service example shows how the missing predictions have direct uses in the future.
- The self-driving car & secondary diagnosis examples shows how the missing predictions may be used under a failure mode.
- The LLM example shows how missing predictions may be utilized for the assessment of internal biases.

Comparison with Existing Evaluation Metrics

The counterfactual score $\psi = \mathbb{E}[S]$ can be decomposed in the following way:

 $\psi = \mathbb{E}[S | R = 0]\mathbb{P}(R =$

The first term is a product of the selective score and coverage (second term is ignored).

Condessa et al. (2017) proposes the classification quality score θ , assuming $S \in [0, 1]$:

 $\theta = \mathbb{E}[S \mid R = 0]\mathbb{P}(R = 0) + \mathbb{E}[1 - S \mid R = 1]\mathbb{P}(R = 1).$

This would **penalize** abstaining on good predictions, which is not ideal in our applications. But it can also be estimated given our tools, as $\theta + \psi$ is an observable quantity.

$$= 0) + \mathbb{E}[S | R = 1]\mathbb{P}(R = 1).$$

Simulated Experiment: Data & Predictions



Simulated Experiment: Full Results

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



Two abstaining classifiers, depicted using their decision boundary (orange), predictions (\bullet/\blacktriangle) , and abstentions (x).

> With sufficiently flexible nuisance learners, DR CI achieves the correct miscoverage rate (small bias), and its width is half the width of the IPW CI (small variance).

$\hat{\pi}$ / $\hat{\mu_0}$	95% Cl's	Plug-in	IPW	DR
inear/Logistic	Miscoverage	1.00	0.76	1.00
	Width	0.00	0.09	0.04
andom Forest	Miscoverage	0.64	0.14	0.05
	Width	0.02	0.13	0.07
ouper 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.





Details for the CIFAR-100 Experiment

softmax response (SR) (at 0.8 vs. 0.5).

- similar examples and their scores on abstentions happen to be similar).

- Note: First half (5,000) of the "test set" is used to train the output layers.

• Scenario I: same base classifiers (pre-trained VGG-16) & different thresholds for the

 $SR(\mathbf{p}) = \max_{c \in [C]} p_c.$

• Note that these are deterministic abstention rules (still works, as the two happen to abstain on

• Scenario II: same base classifiers & different stochastic abstention rules (SR vs. Gini).

• Scenario III: different base classifiers (1 vs. 2 output layers) & same abstention rules (SR).

Asymptotic Confidence Sequences for Counterfactual Scores

- abstaining classifiers in an anytime-valid manner (i.e., at arbitrary stopping times).
- precise approximation to a non-asymptotic CS, as $n \rightarrow \infty$.

 $o_{a.s.}(\sqrt{n^{-1}\log\log n})$ rate, then, for each $\alpha \in (0, 1)$,

$$C_{n} := \left(\hat{\psi}_{dr} \pm \sqrt{\hat{Var}_{n}(\hat{IF})} \sqrt{n^{-2}(2n\hat{\sigma}_{n}^{2} + 1) \cdot \log\left(\alpha^{-1}\sqrt{n\hat{\sigma}_{n}^{2} + 1}\right)} \right)$$

where $\hat{\sigma}_{n}^{2}$ is the variance estimate of $\hat{\psi}_{n}$.

• Leveraging the recent results by Waudby-Smith et al. (2021), we can further estimate the counterfactual scores of

• Informally, an asymptotic confidence sequence (AsympCS) refers to a sequence of intervals that is an arbitrarily

Theorem. Let $\psi = \mathbb{E}[S]$ be the counterfactual score of an abstaining classifier. Assume an (i.i.d.) test set $\{(X_i, Y_i)\}_{i=1}^n$. Also, let $\hat{\psi}_{dr}$ be the DR estimator. If the nuisance functions for $\hat{\psi}_t$ are estimated at a product

forms a $(1 - \alpha)$ -level AsympCS for ψ .



End of Slides