

# Discussion

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We congratulate the authors on these illuminating and thought-provoking articles.

## 1. SCORING RULES AND WELL-SPECIFICATION IN PREDICTIVE MODELING

In the context of prediction, the objective is often to minimize a particular criterion or scoring rule. If the conditional distribution is known and correctly specified, then maximum likelihood is the criterion that should be used for estimation, even if the Kullback-Leibler divergence is not the scoring rule that the forecaster has chosen to minimize. In the more likely case of misspecification, it is not clear which criterion should be used for estimation. In the context of forecasting conditional probabilities of binary outcomes, [Elliott et al. \(2016\)](#) examine this question and illustrate that the choice of scoring rule yields different best approximations to the true conditional probability function of the outcome of interest under misspecification, except under restrictive conditions. Interestingly, these conditions under which the choice of objective function used for estimation does not change the best approximation to the true conditional probability function imposes symmetry conditions on the regressor distribution as well as the conditional mean.

## 2. CAUSAL INFERENCE, WELL-SPECIFICATION AND EXTERNAL VALIDITY

In causal inference, we often consider fully nonseparable models. For simplicity, we will consider the case where  $\vec{X} = T$ , where  $T$  is a scalar binary variable, which we refer to as the treatment variable. The model equation is specified as

$$(1) \quad Y = m(T, \vec{U}).$$

In this simple example, the structural function could be written in terms of potential outcomes ([Imbens and Rubin 2015](#)),

$$(2) \quad Y = (1 - T)Y_0 + TY_1,$$

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\*This material is based upon work supported by the National Science Foundation under Grant No. DMS 1712940.

where  $Y_0 = m(0, \vec{U})$  and  $Y_1 = m(1, \vec{U})$ . We can also write the conditional distribution of  $Y$  given  $T$  in terms of the potential outcomes,

$$(3) \quad F_{Y|T}(y|t) = \int 1\{m(t, \vec{u}) \leq y\} dF_{\vec{U}|T=t} = F_{Y_t|T}(y|t), \quad \text{for } t = 0, 1.$$

Due to potential selection,  $\vec{U}$  may not be independent of  $T$  in general. In this case, we cannot identify the average treatment effect (ATE), i.e.

$$(4) \quad \Delta(P) = E_P[Y_1 - Y_0] = \int (m(1, \vec{u}) - m(0, \vec{u})) dF_{\vec{U}},$$

from the observed difference in mean outcomes,

$$(5) \quad E_P[Y|T=1] - E_P[Y|T=0] = \int m(1, \vec{u}) dF_{\vec{U}|T=1} - \int m(0, \vec{u}) dF_{\vec{U}|T=0}.$$

Hence, the independence of  $U$  and  $T$  are critical, i.e.  $F_{\vec{U}|T} = F_{\vec{U}}$ , for the identification of the ATE in (4) from the difference in mean outcomes in (5).

Randomized experiments or randomly assigned interventions ensure this independence assumption holds and thereby allow us to learn about *internally valid* estimands of causal impact, such as the ATE. In general, these estimands may not be *externally valid* (for further discussion of the distinction between internal and external validity, see [Athey and Imbens 2017](#)). For instance, the ATE in a given experiment can depend on the environment. To allow for this dependence in our notation, let  $e \in \mathcal{E}$  denote an environment, then

$$(6) \quad Y^e = m^e(T^e, \vec{U}^e),$$

$$\Delta^e(P^e) = E_{P^e}[Y_1^e - Y_0^e] = \int (m^e(1, \vec{u}^e) - m^e(0, \vec{u}^e)) dF_{\vec{U}^e},$$

where  $\Delta^e(P^e)$  denotes the ATE for the environment  $e$ . Note that every function in the above may vary with  $e$ . The above notation also clarifies that while the independence between  $T$  and  $\vec{U}^e$  ensures that we identify the ATE for the environment  $e$ , i.e. an internally valid estimand, it is not sufficient for  $\Delta^e(P^e) = \Delta_0$  for all  $e \in \mathcal{E}$ , a non-singleton set.

The authors point to an interesting connection between well-specification in the context of causal inference and invariance to regressor distributions ([Peters et al. 2016](#)). We conjecture that this connection relates to external validity. We provide a simple example to support our conjecture. To do so, we present the assumptions maintained in [Peters et al. \(2016\)](#), while adapting their notation slightly to remain consistent with ours. We observe i.i.d. realizations of  $(X^e, Y^e)$  in each environment, where  $X^e \in \mathbb{R}^p$  and  $Y^e \in \mathbb{R}$  is the target variable. [Peters et al. \(2016\)](#) assume that if a subset  $S^* \subseteq \{1, \dots, p\}$  is causal, then

$$(7) \quad Y^e = g(\vec{X}_{S^*}^e, \vec{\epsilon}^e), \quad \vec{\epsilon}^e \sim F_{\vec{\epsilon}}, \quad \vec{\epsilon}^e \perp \vec{X}_{S^*}^e.$$

The goal of [Peters et al. \(2016\)](#) is to use different types of interventions in different environments for causal identification. Here we will apply their assumption to our treatment effect problem, where we only consider interventions that randomly

assign  $T^e$  within each environment, i.e.  $T^e \perp (\vec{Z}^e, \epsilon^e)$  for all  $e \in \mathcal{E}$ . To do so, we let  $\vec{X}^e = (T^e, \vec{Z}^e)'$ , assuming (7) implies that

$$(8) \quad Y^e = g\left(\left(T^e, \vec{Z}^e\right)', \epsilon^e\right).$$

We can identify the following

$$(9) \quad E_{P^e} \left[ Y_1^e - Y_0^e | \vec{Z}^e = \vec{z} \right] = \int (g((1, \vec{z}')', v) - g((0, \vec{z}')', v)) dF_{\epsilon}(v) = CATE(\vec{z}),$$

which is the conditional average treatment effect given  $\vec{Z}^e = \vec{z}$ . As we can see from the first equality, this object does not vary across environments. Hence, it is not only internally but also externally valid for  $e \in \mathcal{E}$ . This is not surprising, since (7) assumes that the function  $g$ , the distribution of unobservables  $F_{\epsilon}$  and the regressors  $\vec{Z}^e$  are the same across environments, even though the distribution of  $\vec{Z}^e$  can vary arbitrarily across environments.

Even though in the above example  $CATE(\vec{z})$  is externally valid, we can easily show that this is not true for the ATE. To see this, note that

$$(10) \quad \Delta^e(P^e) = \int CATE(\vec{z}) dF_{\vec{Z}^e}(\vec{z}).$$

It clearly varies across environments depending on the distribution of  $\vec{Z}^e$ . Hence, it is not externally valid.

This simple example supports our conjecture that the relationship between the invariance principle introduced in these papers is indeed related to the concept of external validity. We thank the authors for this important insight.

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