Model-Robust Counterfactual Prediction Method

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Abstract—We develop a method for assessing counterfactual predictions with multiple groups. It is tuning-free and operational in high-dimensional covariate scenarios, with a runtime that scales linearly in the number of datapoints. The computational efficiency is leveraged to produce valid confidence intervals using the conformal prediction approach. The method is model-robust in that it enables inferences from observational data even when the data model is misspecified. The approach is illustrated using both real and synthetic datasets.

Index Terms—counterfactuals, causal inference, conformal prediction

I. INTRODUCTION

In many casual inference problems, the subject or unit of analysis belongs to a group, indexed by $z$, and is associated with a continuous outcome (or response) $y$. For instance, groups $z \in \{0,1\}$ may correspond to ‘not receiving’ or ‘receiving’ medication. The inferential question is then typically posed in counterfactual terms:

“What would the outcome have been, had the unit belonged to a different group $\tilde{z} \neq z$?”

The ability to address this question using observational data is relevant in a wide variety of fields, including clinical trials, epidemiology, econometrics, policy evaluation, etc. [1]

Each unit is typically associated with a range of covariates (or features), collected in a vector $x$, which may affect its outcome and/or group selection. When $x$ contains all variables that simultaneously affect both $y$ and $z$, it is possible to provide causal interpretations from observed data. The onus is on the researcher to include such potentially confounding variables [2]. Under this standard condition, the dependencies between group, outcome and covariates can be encoded by a graph as in Figure 1 along with an associated joint distribution $p(x, y, z)$.

![Dependency graphs](image)

Fig. 1: Dependency graphs, where ● and ■ represent random and deterministic variables, respectively. Left: Observed outcome. Right: Counterfactual outcome when assigning group $\tilde{z}$.

The counterfactual question above can now be directly translated into predicting the counterfactual (or potential) outcome, $y(\tilde{z})$, had the unit been set to $\tilde{z}$, thus overriding the covariate-dependency of the group assignment $\tilde{z}$. The resulting dependencies for $y(\tilde{z})$ can also be encoded in a graph shown in Figure 1 with an associated joint distribution $p(x, y(\tilde{z}), z)$ [1], [9]. Since it follows that $p(y(\tilde{z})|x) = p(y|x, z = \tilde{z})$, the counterfactual outcome $y(\tilde{z})$ can be predicted by the conditional mean

$$\mu_{\tilde{z}}(x) = \mathbb{E}[y|x, z = \tilde{z}].$$

This target quantity can be learned using observed data from $n$ units:

$$\mathcal{D} = \{(x_1, y_1, z_1), \ldots, (x_n, y_n, z_n)\},$$

assuming that the units are drawn independently from the data generating process $p(x, y, z)$ and that there is an overlap of covariates in all groups $p(z|x) > 0$ [10].

In most prior works, the targeted quantity has been the difference between means, that is,

$$E[y(1)|x] - E[y(0)|x] = \mu_1(x) - \mu_0(x), \quad (1)$$

but after averaging out the covariates $x$, cf. [2], [11]. Many methods that estimate this target quantity, model either the outcome of each group or the group selection mechanism as functions of $x$. Much effort has been made to formulate model-robust methods as well as extending them to the case of high-dimensional $x$ so as to include more potential confounders, cf. [12]–[15].

For the counterfactual question above, it is however more relevant to compare the covariate-specific predictions directly, rather than averaging them over $x$, cf. [16]–[18]. This is the focus of several methods based on fitting flexible predictive models from statistical machine learning, such as decision trees [19], [20] and deep neural networks [21]. One limitation of targeting the difference between predictions is that the dispersions of the counterfactual outcomes are omitted. While correctly inferring that, say, $\mu_1(x) < \mu_0(x)$, it may still be the case that $y(1)$ frequently exceeds the value of $y(0)$. Such considerations are important in applications where different groups involve differential risks. Then reporting the difference [11] alone omits valuable information.

The dispersion of outcomes around the prediction $\mu_{\tilde{z}}(x)$ can be quantified by a prediction interval $C_2(x)$ in a straightforward manner if the variance function $\text{Var}[y|x, z = \tilde{z}]$ were known. Since both mean and variance functions are unknown, the challenge here is to provide model-robust predictions and intervals. We develop a counterfactual prediction method with the following key features:

1Eq. [1] is often called ‘conditional average treatment effect’ (CATE) and ‘average treatment effect’ (ATE) after marginalizing out $x$. 

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it produces prediction intervals that are statistically valid, even under model misspecification and with finite number of samples \( n \),

- it takes into account the outcome dispersions in each group, and therefore targets a different level of inferences than the difference of averages in (1).

- it is operational even in the undersampled case, that is, when the number of covariates in \( x \) exceeds \( n \),

- it performs variable selection within each group by pruning out covariates in \( x \) that have no effect on the outcome,

- it does not require cross-validation or other tuning techniques and is computationally efficient.

The method builds upon results in the conformal prediction literature \([22]\) and online sparse learning \([23]\).

**Notation:** \( ||\cdot||_1 \) and \( ||\cdot||_2 \) denote the \( \ell_1 \) and \( \ell_2 \)-norms, respectively. \( \ominus \) denotes the element-wise Hadamard product.

**Remark:** Code for the proposed method available at https://github.com/dzachariah/counterfactual

### II. Counterfactual Predictions

Consider a unit with covariates \( x \) and let \( C_{0,\beta}(x) \) denote a finite interval that covers the outcome

\[
y \in C_{0,\beta}(x) \quad \text{when} \quad z = 0,
\]

with a probability of at least \( \beta \). We define \( C_{1,\beta}(x) \) in a similar manner for group \( z = 1 \). See Figure 2 for an illustration.

Based on the standard dependency assumptions considered in the previous section, we will assess the counterfactual effect of group \( \bar{z} \) on units with covariates \( x \), by comparing the prediction intervals.

The above reasoning is readily generalized into a framework with multiple groups \( z \in \{0, \ldots, K - 1\} \). Using a subset of the observed data,

\[
D_z = \{(x_i, y_i)\}, \quad \text{where} \quad (x_i, y_i) \sim p(x, y \mid z = \bar{z}),
\]

our aim is to obtain a point prediction \( \hat{\mu}_z(x) \) and an interval \( C_{z,\beta}(x) \) with valid coverage properties, even when lacking a correctly specified model of the data generating process \( p(x, y, z) \). This provides a model-robust means of evaluating the effects of the groups that is complementary to evaluating just the differences between predictions.

**Example:** Consider an observational study with \( K = 3 \) groups and a scalar covariate \( x \), as illustrated in Fig. 3. Using the method described in the subsequent section, we form \( \hat{\mu}_z(x) \) and the corresponding prediction intervals \( C_{z,\beta}(x) \), for a given \( x \) and all groups \( z \in \{0, 1, 2\} \). The plots enable an intuitive assessment of both the size and significance of the effects of each group.

**Definition II.1.** Given \( x \), the predicted outcome for group \( \bar{\bar{z}} \neq z \) is **counterfactually significant** if the prediction intervals do not overlap. That is, they are mutually exclusive

\[
C_{\bar{z},\beta}(x) \cap C_{z,\beta}(x) = \emptyset. \tag{2}
\]

The prediction is said to have 100\( \beta \)% **counterfactual confidence**, where \( \beta \) is the largest value for which (2) holds. Note that the definitions are symmetric with respect to all pairs of groups. They take into account the dispersions of each group, unlike measures such as (1).

**Example, cont’d:** In Fig. 3 we see that for a unit with covariate \( x = -1 \), the counterfactual confidence group of 1 relative to group 2 is greater than 90%. The confidences for the counterfactual predictions are tabulated pairwise below for covariate \( x = -1 \) (left) and \( x = 2 \) (right):

| \( \bar{z} \) | 0 | 1 |
|---|---|---|
| 1 | 81% | - |
| 2 | 64% | 96% |

| \( \bar{z} \) | 0 | 1 |
|---|---|---|
| 1 | - | 24% |
| 2 | 45% | 58% |

It is seen that for \( x = -1 \), the inferred effects of \( \bar{z} \) can be asserted with greater confidence than for \( x = 2 \). This is corroborated by comparing the datasets shown in Fig. 3.

### III. Counterfactual Prediction Method

Starting from the perspective of counterfactual predictions outlined above, we now develop a method for obtaining \( \hat{\mu}_z(x) \) and \( C_{z,\beta}(x) \). We begin by considering a regression model class

\[
\mathcal{M}_\mu = \{ \mu : \mu(x) = \phi^\top(x)w, \ w \in \mathbb{R}^p \},
\]

parameterized by \( w \) and where \( \phi(x) \) is a \( p \)-dimensional regressor vector discussed in Subsection III-C. When the model class is well-specified it includes the unknown mean function \( \mu_z(x) \in \mathcal{M}_\mu \).

**A. Learning method**

To learn a model in \( \mathcal{M}_\mu \) from data \( D_z \), we build upon the convex SPICE-method \([23]\), for which the learned weights are given by

\[
\hat{w} = \arg\min_w \|y - \Phi w\|_2 + \|\varphi \odot w\|_1, \tag{3}
\]

where \( y \) is the vector of observed outcomes and \( \Phi \) is the matrix of regressors with \( \ell \)th row \( \phi^\top(x) \). The elements of \( \varphi \) are given by

\[
\varphi_{j} = \begin{cases} 
\frac{1}{\sqrt{|D_j|}} \| \Phi_j \|_2, & j > 1 \\
0, & \text{otherwise}.
\end{cases}
\]

The learning method (3) is globally convergent, tuning-parameter free and employs an adaptive regularization that
mitigates overfitting. The regularization leads to sparse solutions and therefore performs covariate selection with a predictive performance that can be related to the best subset predictor, see [22] for more details. In addition, [3] can be computed sequentially with a runtime that is linear in the number of samples, $O(|D_z|^2)$. This computational property is leveraged to produce tractable and model-robust prediction intervals.

B. Prediction intervals

The principle of conformal prediction can be described as follows [23]: For the covariate of interest $x$, consider a new sample $(x, \tilde{y})$ where $\tilde{y}$ is a variable. Then quantify how well this sample conforms to the observed data $D_z$ via the learned model (3). All points $\tilde{y}$ that conform well, form a prediction interval.

The conformity is quantified by including $(x, \tilde{y})$ in the learned model (3), which achieved by a sequential update in $O(p^2)$. Then, following [24], we define a measure

$$\pi(\tilde{y}) = \frac{1}{|D_z| + 1} \left(1 + \sum_i I\{r_i \leq |\tilde{y} - \phi^T(x)\hat{w}_i|\right),$$

where $r_i = |y_i - \phi^T(x_i)\hat{w}|$ is the $i$th fitted residual and $I\{\cdot\}$ is the indicator function. The measure is bounded between 0 and 1, where lower values correspond to higher conformity. We construct $C_{z,\beta}(x)$ by varying $\tilde{y}$ over a set of grid points $\tilde{Y}$, as summarized in Algorithm 1. By leveraging the computational properties of the learning method, the prediction interval is computed with a total runtime of $O(|\tilde{Y}|p(p+|D_z|))$. The range of $\tilde{Y}$ is set to exceed that of the outcomes in the observed dataset. A point prediction $\hat{\mu}_z(x)$ is obtained as the minimizer of $\pi(\tilde{y})$.

Algorithm 1: Conformal prediction interval

1: Input: covariate $x$, target coverage $\beta$ and data $D_z$
2: for all $\tilde{y} \in \tilde{Y}$ do
3: \quad Update $\hat{w}$ using $(x, \tilde{y})$
4: \quad Compute $\{r_i\}$ and $\pi(\tilde{y})$ in (4)
5: end for
6: Output: $C_{z,\beta}(x) = \{\tilde{y} \in \tilde{Y} : (n+1)\pi(\tilde{y}) \leq \lceil \beta(n+1) \rceil\}$

Despite the fact that no dispersion model of the data generating process is required, the resulting prediction intervals exhibit valid coverage properties. If the unknown mean function $\mu_z(x)$ belongs to the model class $\mathcal{M}_\mu$, the interval exhibits asymptotic conditional coverage, that is,

$$\Pr\{y \in C_{z,\beta}(x) \mid x, z\} = \beta + o_P(1),$$

under certain regularity conditions [24 thm. 6.2]. More generally, $C_{z,\beta}(x)$ is calibrated to ensure marginal coverage [24 thm. 2.1]

$$\Pr\{y \in C_{z,\beta}(x) \mid z\} \geq \beta.$$

Note that this does not require a well-specified model class $\mathcal{M}_\mu$. In other words, the more accurate the learned regression model, the tighter the prediction interval but its validity remains not matter if the model is correct or not. This confers a robustness property to the proposed inference method in cases when $\mu_z(x) \notin \mathcal{M}_\mu$.

C. Regression models

We consider two simple regression models that minimize or eliminate the need for user input. Suppose $x$ contains $d$ covariates, which can be continuous, discrete, or mixed. The default regressor type is a simple linear function:

$$\phi(x) = \text{col}\left\{1, x\right\}. \quad (5)$$

The regressor (5) has dimension $p = d + 1$. However, by modeling nonlinear effects, one can often obtain tighter prediction intervals. When $x$ contains a smaller number of continuous covariates denoted $x'$ (and the remaining covariates $x''$ are discrete), we suggest a second regressor type

$$\phi(x) = \text{col}\left\{1, \tilde{\phi}_1(x'_1), \ldots, \tilde{\phi}_d(x'_d), x''\right\}, \quad (6)$$

where $\tilde{\phi}_j(x'_j)$ denotes an $m$-dimensional subvector for each dimension of $x'$. Specifically, we use a basis expansion with excellent approximation properties [28], where the $k$th term of $\tilde{\phi}_j(x'_j)$ is given by:

$$\frac{1}{\sqrt{L_j}} \sin\left(\frac{\pi k(x'_j - \bar{x}_j)}{2L_j}\right), \quad k = 1, \ldots, m,$$

where $\bar{x}_j$ denotes the sample mean and $L_j$ is the maximum deviation from the mean (both are obtained from $D$). The regressor (6) has dimension $p = md_0 + d_1 + 1$, where $d_0$ and $d_1$ denote the number of continuous and discrete covariates, respectively.
IV. Numerical experiments

In this section we demonstrate the proposed counterfactual prediction approach by means of three examples. In the following examples, we consider $K = 2$ groups.

A. Nonlinear effects

To illustrate the use of the nonlinear regression function (6), we consider the example in [19] where the data is generated as follows. For each unit, a group $z$ is assigned with equal probability. Then the covariate $x$ (with $d = 1$) is drawn as

$x | (z = 0) \sim \mathcal{N}(40, 10^2)$ and $x | (z = 1) \sim \mathcal{N}(20, 10^2)$

and the counterfactual outcomes as

$y(0)|x \sim \mathcal{N}(72 + 3\sqrt{|x|}, 1)$ and $y(1)|x \sim \mathcal{N}(90 + \exp(0.06x), 1).$ (7)

A simulated observational dataset $\mathcal{D}$ with $n = 120$ is illustrated in Fig. 4. To obtain the predictions in the figure, we use $m = 8$ in [6]. For a unit with covariate $x = 30$, as an example, we note that $\hat{\mu}_1(30)$ is larger than $\hat{\mu}_0(30)$ and that both confidence intervals are tight, as is expected by inspecting the data generating process (7) at the given covariate. In addition, the counterfactual confidence is found to be greater than 90%.

To illustrate the robustness property of the prediction intervals, we repeat the experiment using 1000 Monte Carlo simulations. For each simulation, we generate new data $\mathcal{D}$ and also draw a new unit from both groups. For a unit in group $z = 0$, the outcome is found to belong to interval $C_{0,\beta}(x)$ with probability 0.931 when $\beta = 1$. Similarly, for group $z = 1$, the outcome is contained in the interval $C_{1,\beta}(x)$ with probability 0.905. This coverage property holds even though the predictions relied on a misspecified model (6).

B. High-dimensional covariates

The desire to include all potential confounders in the covariate vector $x$, may lead in many applications to dimensions $d$ that can be larger than $n$ [14]. To address this issue, we simulate an experimental setting with $\Sigma$ constructed using outer products of Gaussian vectors. This generates highly correlated covariates, as is typical in real applications. The counterfactual outcomes are generated as

$y(0)|x \sim \mathcal{N}(x_1 + 5x_{10} + 5x_{20} + 0.5, 0.5^2)$ and $y(1)|x \sim \mathcal{N}(x_1 + x_{10} - x_{30}, 0.5^2).$ (8)

However, this is not a problem for the learning method which automatically prunes away irrelevant covariates due to the adaptive regularization in [4].

A simulated observational dataset $\mathcal{D}$ is shown in Fig. 5. We also illustrate the predicted outcomes for a unit with all covariates equal to one, $x = 1$. We observe that $\hat{\mu}_0(1)$ is considerably larger than $\hat{\mu}_1(1)$, also when taking into account the prediction intervals. This is consistent with the data generating process (8) evaluated at the fixed $x$. The interval for group $z = 0$ is also seen to be significantly wider than that for group $z = 1$, reflecting the larger uncertainty of the predicted outcome. In this case it is possible to assert counterfactual confidence greater than 90%.

We repeat this experiment as well to validate the coverage properties of the intervals, using 1000 Monte Carlo simulations. For each simulation, we generate new data $\mathcal{D}$ and also draw a new unit from both groups. For a unit in group $z = 0$, the outcome is found to be contained in interval $C_{0,\beta}(x)$ with probability 0.921 when $\beta = 0.9$. Similarly, for group $z = 1$, the outcome is contained in the interval $C_{1,\beta}(x)$ with probability 0.915.

C. Schooling data

Following the example in [20], we assess the effect of schooling on income for adults in the US born in the 1930s, using data from [27]. The observed outcome $y$ is the weekly earnings (on a logarithmic scale) of a subject in 1970. Each subject belongs to one of two groups: $z = 1$ corresponds to receiving 12 years of schooling or more and $z = 0$ corresponds to receiving less than 12 years. We consider 26 discrete covariates in $x$. Ten covariates indicate the year of birth 1930-1939, and eight indicate the census region. In addition, eight indicators represent ethnic identification, marital status and whether or not the subject lives in the central city of a metropolitan area. The observational study consists of $n = 329,509$ samples. (See [26] for details.)

Discrete covariates can be partitioned into separate subclasses, and a direct inference approach would be to estimate the average outcomes of groups 0 and 1 for each class. However, the number of classes grows quickly and there are not sufficient samples in the dataset $\mathcal{D}$ for each class and group. Therefore we apply the proposed method, using the regression function (5). The predicted effects of schooling on income are illustrated for subjects in different covariate classes in Fig 6. All subjects in these classes were born in the same year and came from the same region. The prediction interval widths are likely to be affected by the very coarse division of schooling used here, since $z = 0$ includes 0 to 11 years of schooling, which is a substantial variation, while $z = 1$ includes 12 years and more.

The three classes are $x_1$: Caucasian, unmarried and not in a major city, $x_2$: Caucasian, married and in a major city, and $x_3$: African-American, married, and in a major city. Given that the units are logarithmic, the differences of predicted earnings, $\hat{\mu}_1(x) - \hat{\mu}_0(x)$, correspond to +52%, +26% and +39% of weekly earnings, for $x_1$, $x_2$ and $x_3$, respectively. This means that the inferred effect of schooling is greatest for $x_1$ while considerably less for $x_2$. The prediction intervals in Fig. 6 suggest, however, that there is a considerable dispersion of the outcome around the predictions. The predicted outcome
of schooling has a counterfactual confidence of 33%, 20% and 25% for the three cases. Thus for class $x_2$, the predicted gains from schooling are not only the lowest but also have the weakest significance.

The findings appear to be consistent with features of US society in the 1970s: a Caucasian person in a major city with a family was expected to have greater access to economic opportunities, such that schooling experience mattered less to earnings. For the unmarried counterpart who lived outside of the major city, such alternative opportunities were fewer so that schooling could have a more significant impact. An African-American person in a major city with a family represents an intermediate case.

V. CONCLUSIONS

We have developed an inference framework for assessing counterfactuals using prediction intervals for multiple groups. The proposed inference method does not require the tuning of any user-parameters, is computationally efficient, and operational even when the number of covariates exceeds the number of samples. Moreover, the method is model-robust in that the prediction intervals are statistically valid, even without a correct specification of the data model. We demonstrated the method using both real and synthetic data.

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Fig. 6: Inferred effect of schooling on weekly earnings (in logarithmic units) using 90%-prediction intervals. Left: Caucasian, unmarried and not in major city. Center: Caucasian, married and in city. Right: African-american, married and in city.

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