Conditionality principle under unconstrained randomness

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Abstract

A very simple example demonstrates that Fisher's application of the conditionality principle to regression ("fixed-x regression"), endorsed by David Sprott and many other followers, makes prediction impossible in the context of statistical learning theory. On the other hand, relaxing the requirement of conditionality makes it possible via, e.g., conformal prediction.

Contents

1 Introduction

The main goal of this note is to draw the reader's attention to the fact that the conditionality principle is not compatible with statistical learning theory, in which the task is to predict the label y of an object x. Two characteristic features of statistical learning theory are that the labelled objects (x, y) are only assumed to be independent and identically distributed (the unrestricted *assumption of randomness*) and that the objects x are complex (such as videos), so that we are unlikely to ever see identical objects. These two features make prediction impossible if we want to condition on the observed sequence of xs as recommended by Fisher. This is not a new observation, but it might not be as widely known as it deserves.

2 Assumption of randomness and conformal prediction

In statistical learning theory (see, e.g., [18, 17]) we consider *observations* (x, y) each consisting of two components: an *object* $x \in \mathbf{X}$ and its *label* $y \in \mathbf{Y}$. In general, the *object space* $\mathbf{X}$ and *label space* $\mathbf{Y}$ are arbitrary measurable spaces, but to discuss the relevance to Fisher's ideas it will often be convenient to concentrate on the case of *regression* $\mathbf{Y} = \mathbb{R}$.

The simplest setting is where we are given a training sequence

$$(x_1, y_1), \ldots, (x_n, y_n)$$

and the problem is to predict the label y_{n+1} of a test object x_{n+1}. The (unrestricted) *assumption of randomness* is that the observations $(x_1, y_1), \ldots, (x_{n+1}, y_{n+1})$ are generated independently from an unknown probability measure on $\mathbf{X} \times \mathbf{Y}$. This assumption is standard in machine learning and popular in nonparametric statistics.

One way to make predictions with validity guarantees under unconstrained randomness is *conformal prediction* [2, 19]: given a target probability of error $\epsilon > 0$ conformal prediction produces a prediction set $\Gamma \subseteq \mathbf{Y}$ such that $y_{n+1} \in \Gamma$ with probability at least $1-\epsilon$. The basic idea of conformal prediction is familiar (see, e.g., [7, Sect. 7.5]): we fix a statistical test of the null hypothesis of randomness, go over all possible labels y for the test object x_{n+1}, and include in Γ all labels y for which the augmented training set $(x_1, y_1), \ldots, (x_n, y_n), (x_{n+1}, y)$ does not lead to the rejection of the null hypothesis. In many interesting cases this idea has computationally efficient implementations (see, e.g., [19, Sects. 2.3 and 2.4], [2, Sect. 9.2], and [13]).

3 A simple conditionality principle and example

In this section we will only need a special case of the conditionality principle, which I will call the "fixed-x principle" partly following Aldrich [1]. The fixed-x

principle says that, when performing any kind of statistical analysis, we should consider the observed sequence of objects $x_1, \dots, x_{n+1}$ as fixed, even if they were in fact generated from some probability distribution (known or unknown). This is applicable to regression problems (*fixed-x regression*), or any other prediction problems of the kind described in the previous section.

Fisher was a life-long promoter of both the general conditionality principle (which was introduced formally only in 1962 by Birnbaum [6]) and the fixed-x principle as its special case. When H. Fairfield Smith asked Fisher about the origin of the fixed-x principle (treating "the independent variable as fixed even although it might have been observed as a random sample of some variate population") in his letter of 6 August 1954 [5, pp. 213–214], Fisher responded with a reference to his 1922 paper [8, p. 599].

See Aldrich [1] about the development of Fisher's fixed-x regression. Aldrich quotes Fisher [9, Sect. 2, p. 71] (in the context of regression with y having a Gaussian distribution given x): "The qualitative data may also tell us how x is distributed, with or without specific parameters; this information is irrelevant."

David Sprott, a prominent follower of Fisher's, also promoted the conditionality principle in his work. In his 1989 interview with Mary Thompson [16], he remembers a case when, as a student, he was tempted to take into account the variation in the xs in a practical regression problem. His statistics professor said, "No, you wouldn't do that, you'd condition on the xs". Sprott couldn't find out why conditioning on the xs was the right thing to do until he went to London a few years later to work with Fisher, but then he was fully convinced by Fisher.

The intuition behind the fixed-x principle is that only the observed objects are relevant for predicting the label of x_{n+1}. In Sect. 5 we will discuss this in a wider context. And in this section, we discuss the paralysing effect of the fixed-x principle under unrestricted randomness using the following example.

Example 3.1. Consider the problem of regression with $\mathbf{X} = \mathbf{Y} = \mathbb{R}$, and suppose:

- the training sequence is such that $y_i = x_i$ for all $i = 1, \dots, n$, for a large n;
- $x_1, \dots, x_{n+1}$ are all different.

What can we say about y_{n+1} knowing x_{n+1}?

Example 3.1 may describe a situation where the observations are independent and coming from the same continuous distribution. Under the assumption of randomness, we can confidently claim that $y_{n+1} = x_{n+1}$; otherwise, the last observation looks strange and leads to a p-value of $1/(n+1)$ for a fixed statistical test. As the test statistic T for such a test we can take, e.g.,

$$T := \begin{cases} 1 & \text{if } |y_{n+1} - x_{n+1}| > |y_i - x_i|,\ i = 1, \dots, n, \\ 0 & \text{otherwise.} \end{cases}$$

For any $\epsilon \geq 1/(n+1)$, we have $[x_{n+1}, x_{n+1}]$ as the prediction interval for y_{n+1} at confidence level $1 - \epsilon$. Intuitively, this follows from the expectation that the future will be similar to the past (Laplace's rule of succession). Conformal prediction extends this idea greatly.

However, we can say nothing whatsoever about y_{n+1} if we condition on the observed $x_1, \dots, x_{n+1}$. The problem with conditioning on x is that it destroys the assumption of randomness. The assumption of randomness becomes the following *assumption of conditional randomness*: the data-generating distribution P is determined by an arbitrary sequence $(x_1, \dots, x_{n+1}) \in \mathbf{X}^{n+1}$ and an arbitrary family of probability measures $\{Q_x \mid x \in \mathbf{X}\}$ on $\mathbf{Y}$ (measurable in the sense of being a Markov kernel with $\mathbf{X}$ as source and $\mathbf{Y}$ as target); we then have $P = (\delta_{x_1} \times Q_{x_1}) \times \dots \times (\delta_{x_{n+1}} \times Q_{x_{n+1}})$, where δ_x is the distribution on $\mathbf{X}$ that is concentrated at x. When $x_1, \dots, x_{n+1}$ are all different, the true conditional distribution of y_{n+1} can be any probability measure on $\mathbf{Y}$ as there are no restrictions on $Q_{x_{n+1}}$.

4 Different kinds of conditionality

In this section I will briefly describe a couple of results that shed light on the phenomenon illustrated by Example 3.1. But let me first embed the fixed-x principle in a more general picture.

In conformal prediction, a common goal is to achieve *conditional validity*, i.e., to make the conditional probability of an error, $y_{n+1} \notin \Gamma$ in the notation of Sect. 2, bounded above by a given ϵ. But what should we condition on? Three kinds of conditional validity have been widely studied in conformal prediction (see, e.g., [19, Sect. 4.7.1] or, in greater detail, [2, Chap. 4]):

- in *object-conditional validity*, we condition on x_{n+1} (or on a function thereof, in which case we will talk about *partial object-conditional validity*);
- in *label-conditional validity*, we condition on y_{n+1};
- in *training-conditional validity*, we condition on $x_1, y_1, \dots, x_n, y_n$.

It might be possible to achieve more than one kind of conditional validity at the same time. One such case is the Bayesian setting where, e.g., in addition to the assumption of randomness we postulate a probability measure over the probability measures R generating one observation; under this extra assumption, we can construct efficient prediction sets satisfying training-conditional and object-conditional validity at the same time. But of course, it does not make sense to aim at achieving all three kinds of conditional validity at the same time.

In this note we are interested in a fourth kind of conditional validity, in which we condition on $x_1, \dots, x_{n+1}$. This is a stronger requirement than object-conditional validity, and already the latter is difficult to achieve under unrestricted randomness.

Lei and Wasserman ([14, Lemma 1], [19, Theorem 4.11]) prove a strong negative result assuming that $\mathbf{X}$ is a separable metric space. In the case of regression ($\mathbf{Y} = \mathbb{R}$), they show that a set predictor satisfying the property of object-conditional validity under unrestricted randomness will output, with probability at least $1-\epsilon$, an unbounded prediction set for y_{n+1} provided the test object x_{n+1} is not an atom of the data-generating distribution. Remember that ϵ is the target probability of error, so that the lower bound $1-\epsilon$ means complete lack of efficiency.

Barber et al. [3] show that an efficient set predictor can satisfy partial object-conditional validity that involves conditioning on $x_{n+1} \in \mathcal{X}$ for all sets $\mathcal{X}$ of probability at least δ for a given $\delta > 0$, but essentially the same properties of efficiency and validity are achieved automatically by unconditionally valid predictors, such as conformal predictors (under some regularity conditions).

Despite these negative results, designing conformal predictors that are conditional in a weaker sense is an active area of research, starting from a basic idea of Mondrian conformal prediction ([19, Sect. 4.6], [2, Chap. 4]). Asymptotically, conditional conformal prediction is possible in a very strong sense [14, Theorem 1]. Finite-sample results are mathematically less satisfying but may hold great promise in practice; see, e.g., [15, 4, 10, 11].

5 General conditionality principle and its difficulties

Cox and Hinkley [7, Sect. 2.3(iii)] point out two versions of the conditionality principle, basic and extended. In the basic version, we are given an *ancillary statistic* C, i.e., a random variable with a known distribution, and the conditionality principle says that our analysis should be conditional on the observed value of C. This prescription is very compelling in some cases, such as Cox's famous example of choosing one of two measuring instruments at random and then observing its reading (knowing which instrument has been chosen); see [7, Example 2.33].

The basic version does not imply the fixed-x principle, since the distribution of the xs does depend on the unknown data-generating distribution. In the extended conditionality principle, the unknown parameter is split into two parts, and only one of those parts is of direct interest to us. In the context of the assumption of randomness, the parameter is the probability measure R on $\mathbf{X}\times\mathbf{Y}$ generating one observation. We can typically (see, e.g., [19, Sect. A.4]) split R into the marginal distribution $R_{\mathbf{X}}$ on $\mathbf{X}$ and the conditional distribution Q_x of y given x, for each $x \in \mathbf{X}$; Q is a Markov kernel. Only $Q := \{Q_x \mid x \in \mathbf{X}\}$ is of interest to us in our prediction problem. Then $C := (x_1, \dots, x_{n+1})$ is ancillary for the Markov kernel Q in the following extended sense:

- The distribution of C does not depend on Q (and only depends on $R_{\mathbf{X}}$).
- The conditional distribution of the remaining part of the data $y_1, \dots, y_{n+1}$ given the value of C depends only on Q (and does not depend on $R_{\mathbf{X}}$).

The extended conditionality principle, requiring analysis to be conditional on C, becomes the fixed-x principle when adapted to the assumption of randomness.

Lehmann and Scholz [12, Sect. 1] point out that conditional inference can be less efficient for small samples, although the difference tends to disappear as the sample size increases. However, Example 3.1 is more serious, since it demonstrates a complete failure of the conditionality principle. Another instance of a comparable complete failure of this principle is where the experimental design involves deliberate randomization, as in a random assignment of subjects to treatments in randomized clinical trials [12, end of Sect. 3]. The conditionality principle then forces us to disregard randomization compromising one of the most standard and powerful statistical tools in medicine.

6 Conclusion

This note observes that the extended conditionality principle prevents successful prediction in statistical learning theory, which is the basic setting of machine learning. (Other varieties of machine learning usually make prediction even more difficult; e.g., they may allow different distributions for the training and test observations.) Its main points (which are far from being original) are:

- we should drop the conditionality principle as a requirement but keep it as an ideal goal (which is often partially achievable but more rarely, and then under strong assumptions, fully achievable);
- doing so permits use of methods with unconditional performance guarantees, such as conformal prediction (and these methods automatically satisfy some weak properties of conditional validity [3]);
- when trying to achieve conditionality as ideal goal, we might need to settle for partial, approximate, or asymptotic conditionality;
- it is important to keep in mind other kinds of conditionality, such as training-conditional, object-conditional, and label-conditional validity.

For several results in these directions, see, e.g., [2, Chap. 4] and [19, Sects. 1.4.4, 4.6, 4.7].

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