

Model Class Reliance: Variable Importance Measures for any Machine Learning Model Class, from the “Rashomon” Perspective

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Abstract

Variable importance (VI) tools are typically used to examine the inner workings of prediction models. However, currently available VI measures tend to not be comparable across model types, can obscure implicit assumptions about the data generating distribution, or can give seemingly incoherent results when multiple prediction models fit the data well. In this paper we propose a framework of VI measures for describing how much any model class (e.g. all linear models of dimension p), any model-fitting algorithm (e.g. Ridge regression with fixed regularization parameter), or any individual prediction model (e.g. a single linear model with fixed coefficient vector), relies on covariate(s) of interest. The building block of our approach, Model Reliance (MR), compares a prediction model’s expected loss with that model’s expected loss on a pair of observations in which the value of the covariate of interest has been switched. Expanding on MR, we propose Model Class Reliance (MCR) as the upper and lower bounds on the degree to which any well-performing prediction model within a

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class may rely on a variable of interest, or set of variables of interest. Thus, MCR describes reliance on a variable while accounting for the fact that many prediction models, possibly of different parametric forms, may fit the data well. We give probabilistic bounds for MR and MCR, leveraging existing results for U-statistics. These bounds can be generalized to create finite-sample confidence regions for the best-performing models from any class. We also illustrate connections between MR, conditional causal effects, and linear regression coefficients. We outline a binary search procedure to compute estimates of MCR for any model class, with specific implementations for the class of regularized linear regression models, and for regression models in a reproducing kernel Hilbert space. We then apply MR & MCR in a public dataset of Broward County criminal records to study the reliance of recidivism prediction models on sex and race, with code available at <https://github.com/aaronjfisher/mcr>.

1 Introduction

In statistics and machine learning studies, questions regarding the importance of variables frequently inform the process of determining a regression model or classification model. An analyst may ask: does my specific prediction model depend on a given set of variables in order to predict well? How much, or how little, could another prediction model rely on this variable while still performing well? Does the algorithm I used to select (i.e., train, or learn) my prediction model rely on a given feature? Will these aspects of variable importance generalize beyond my training data? The second of these questions can be especially relevant when there are multiple prediction models that fit the data almost equally well, but function through different mechanisms. This scenario has been termed the “Rashomon” effect (Breiman et al., 2001), inspired by the 1950 Kurosawa film of the same name, in which four witnesses offer different descriptions and explanations for the same encounter.

The questions listed above are often studied using “variable importance” measures. Linguistically however, the term “variable importance” does not imply an obvious context in

which variables are needed. Variables may be considered “important” in the context of a prediction model’s performance (Breiman et al., 2001), a pseudo-true model that minimizes an expected loss (White, 1982; Müller, 2013), an underlying associational structure (e.g. $\mathbb{E}[Y|X]$ for outcomes Y and covariates X), or a causal mechanism. Whether or not an analyst is able to make conclusions about these different contexts will generally depend on the assumptions made (van der Laan, 2006), and there is debate on which context should take priority (Olden et al., 2004; Freedman, 2006; Archer and Kimes, 2008; Díaz et al., 2015). In this paper, we primarily focus on importance in the context of a prediction model, and use terms such as “model reliance” rather than “importance” to clarify this context. As a secondary goal, we discuss additional assumptions that are sufficient to make our results apply to each of the above contexts.

One popular approach for assessing variable importance is to train a model-fitting algorithm twice, first on all of the data, and then again on a copy of the dataset in which the covariates of interest have been removed. The performance of the two resulting prediction models is then compared (Gevrey et al., 2003). While this approach is intuitive, it can result in seemingly incoherent behavior under the Rashomon effect. Specifically, if several prediction models fit the data well, then removing a variable may not substantially change the prediction loss even if the *best* prediction model relies heavily on that variable. Put another way, these methods can identify the strongest performing prediction model with no reliance on a given variable, but they generally do not bound how much *any* well-performing model may rely on that variable. We refer to such methods as measuring the *Algorithm Reliance* on a variable, and explore them further in Section 3.2.

Other approaches for variable importance only address a subset of the questions posed above; in particular, they do not address the “Rashomon” question of how much diversity exists among prediction models that perform well. In the context of Neural Networks, the “Perturb” sensitivity analysis method compares the accuracy of a prediction model before and after adding random noise to a variable (Recknagel et al., 1997; Yao et al., 1998; Scardi

and Harding, 1999; Gevrey et al., 2003). van der Laan (2006) defines variable importance measures based on the change in the conditional expectation of the outcome when the value of a covariate is changed, and uses methods inspired by the causal inference literature to estimate these measures. In recent work, Williamson et al. (2017) define a variable importance measure based on the conditional variance of the outcome given all covariates compared against the conditional variance of the outcome given all covariates except for a subset of interest. Again though, these methods do not inform the “Rashomon” question.

In this paper we propose a taxonomy of variable importance measures to address the questions stated above. The core building block of our framework is *Model Reliance* (MR), which compares a prediction model’s expected loss with its expected loss in a pair of observations in which the covariate of interest has been switched (see Section 3.1 for a specific definition). Our formulation of MR is inspired by the tree-level, permutation-based importance measure of Random Forests (Breiman, 2001; Breiman et al., 2001), but applied at the aggregate model-level and for a general loss function (see Sections 3.1.1 & 4). Expanding on MR, we propose *Model Class Reliance* (MCR) as the upper and lower bounds for how much any well-performing model within a given class relies on a variable of interest. Roughly speaking, MCR addresses the Rashomon problem by bounding the diversity of explanations offered by well-performing prediction models.

Our work is motivated in part by an applied problem in criminal recidivism prediction, where models are commonly used to inform sentencing and parole decisions (Monahan and Skeem, 2016; Picard-Fritsche et al., 2017). We analyze a public dataset of criminal records from Broward County, FL (Larson et al., 2016), which includes covariates on criminal history, age, race and sex. Given a prediction model, we aim to determine how much that model relies on information that would be considered inadmissible, namely race and sex. Given a class of prediction models, we also study the subset of models which predict well. We find that, among linear classifiers with high empirical accuracy, *none rely heavily* on race and sex to achieve this accuracy (see analysis and discussion in Section 6). This result implies

that, given criminal history and age, even if a practitioner using our dataset tried to create an accurate linear model that depended heavily on race or sex, they would be unable to, because no such linear model exists.

MR and MCR are unknown quantities describing the interplay between a model, or a model class, and an unknown population distribution, and must be estimated from data. Accordingly, we provide finite-sample statistical learning theoretic bounds for MR and MCR using results for U-statistics. In many cases these probabilistic bounds can be generalized to finite-sample confidence intervals for arbitrary summary descriptions of best-in-class models. This inference task becomes equivalent to a case-specific optimization problem, depending on the choice of summary description, and inference is feasible whenever the optimization problem is computationally tractable (see Section 3.3.2).

The remainder of this paper is organized as follows. In Section 2 we introduce notation and terminology. In Section 3.1 we present MR, derive a connection to conditional causal effects, and show simplifications for the case of linear models. In Section 3.2, we discuss Algorithm Reliance, as summarized above. In Section 3.3 we introduce MCR, derive finite sample bounds, and outline a binary search procedure to compute estimates of MCR. We also show that similar techniques can be used to create finite-sample confidence intervals for arbitrary descriptions of best-in-class models, or sets of best-in-class models. In Section 3.4 we consider a version of MCR tailored for the case of correlated variables. In Section 4 we review additional related literature, particularly work focusing on permutation-based VI measures and the Rashomon effect. In Section 5 we illustrate the difference between MR, AR, and MCR, in a simulated example. We analyze a public dataset on recidivism in Section 6. Unless otherwise noted, we provide proofs in Section C of the supplement.

2 Notation: models, algorithms, and model classes

For a given vector \mathbf{v} , let $\mathbf{v}_{[j]}$ denote its j^{th} element(s), where $\mathbf{v}_{[j]}$ may also be a vector if j contains more than one index. Let $\mathbf{v}_{[-j]}$ denote all elements of \mathbf{v} except for $\mathbf{v}_{[j]}$. For a given matrix \mathbf{A} , let \mathbf{A}' , $\mathbf{A}_{[i,\cdot]}$, $\mathbf{A}_{[\cdot,j]}$, and $\mathbf{A}_{[i,j]}$ respectively denote the transpose of \mathbf{A} , the i^{th} row(s) of \mathbf{A} , the j^{th} column(s) of \mathbf{A} , and the element(s) in the i^{th} row(s) and j^{th} column(s) of \mathbf{A} .

We consider the case of regression, or classification, between a random outcome variable $Y \in \mathcal{Y}$ and a vector of covariate variables $X = (X_1, X_2) \in \mathcal{X}$, where the covariate subsets $X_1 \in \mathcal{X}_1$ and $X_2 \in \mathcal{X}_2$ may each be multivariate. We are particularly interested in studying how much different models rely on the subset of covariates X_1 to predict Y . We define $Z = (Y, X_1, X_2)$ as the combined random variable of both outcomes and covariates, with $Z \in \mathcal{Z}$. We refer to our dataset as $\mathbf{Z} = \begin{bmatrix} \mathbf{y} & \mathbf{X} \end{bmatrix}$, a matrix composed of a n -length outcome vector \mathbf{y} in the first column, and a $n \times p$ covariate matrix \mathbf{X} in the remaining columns. We refer to the space of all possible samples of size n as \mathcal{Z}^n . Throughout, we assume that observations of Z are *iid*, that $n \geq 2$, and that solutions to $\arg \min$ and $\arg \max$ operations exist whenever optimizing over sets mentioned in this paper (e.g., in Theorem 6, below).

Before continuing, it is important distinguish between our terminology for a model class, a model, a loss function, and a model-fitting algorithm. We use the term *model class* to refer to a prespecified subset $\mathcal{F} \subset \{f \mid f : \mathcal{X} \rightarrow \mathcal{Y}\}$ of the measurable functions from \mathcal{X} to \mathcal{Y} . We refer to member functions f in the set \mathcal{F} as *prediction models*, or simply as *models*, which take a vector of covariates $x \in \mathcal{X}$ as input and return a prediction of $y \in \mathcal{Y}$. In other words, we use the term “model” to refer to a specific prediction function from \mathcal{X} to \mathcal{Y} (Breiman et al., 2001), rather than a set of potential probability distributions for the data. For a function f and covariate vector $x = (x_1, x_2)$, we overload the notation to write $f(x)$ and $f(x_1, x_2)$ interchangeably. Given a sample observation $z = (y, x)$ and a model f , we evaluate the performance of f using a prespecified, real-valued, and nonnegative *loss function*, denoted by L . For example, when $\mathcal{Y} \subset \mathbb{R}$, one common choice of L is the squared error loss $L(f, z) = L(f, (y, x)) = (y - f(x))^2$. We use the term *algorithm* to refer to any procedure

$\mathcal{A} : \mathcal{Z}^n \rightarrow \mathcal{F}$ that takes a dataset as input and returns a model $f \in \mathcal{F}$ as output. For example, an algorithm may select a model $f \in \mathcal{F}$ by minimizing the empirical loss $\sum_{i=1}^n L(f, \mathbf{Z}_{[i, \cdot]})$, or by balancing the empirical loss with regularization or computational costs. We illustrate these terms with two brief toy examples in Section A.1 of the supplement.

3 Framework of importance measures

In this section we present our core technical results, which describe how much a model, a model-fitting algorithm, or a model class, relies on a subset of covariates X_1 .

3.1 Model reliance

To describe the reliance of a fixed model f on the random variable X_1 in a population, we use the notion of a “switched” loss. Let $Z^{(a)} = (Y^{(a)}, X_1^{(a)}, X_2^{(a)})$ and $Z^{(b)} = (Y^{(b)}, X_1^{(b)}, X_2^{(b)})$ be independent random variables, each following the same distribution as $Z = (Y, X_1, X_2)$. Denote realizations of $Z^{(a)}$ and $Z^{(b)}$ by $z^{(a)} = (y^{(a)}, x_1^{(a)}, x_2^{(a)})$ and $z^{(b)} = (y^{(b)}, x_1^{(b)}, x_2^{(b)})$ respectively. Given the realizations $z^{(a)}$ and $z^{(b)}$, let $h_f(z^{(a)}, z^{(b)})$ be the loss of model f on $z^{(b)}$, if $x_1^{(b)}$ was first replaced with $x_1^{(a)}$:

$$\begin{aligned} h_f(z^{(a)}, z^{(b)}) &= h_f((y^{(a)}, x_1^{(a)}, x_2^{(a)}), (y^{(b)}, x_1^{(b)}, x_2^{(b)})) \\ &:= L(f, (y^{(b)}, x_1^{(a)}, x_2^{(b)})). \end{aligned}$$

For a given prediction function f , we wish to know the expectation of this quantity across pairs in the population, $e_{\text{switch}}(f) := \mathbb{E}h_f(Z^{(a)}, Z^{(b)})$. Alternatively, the same population functional $e_{\text{switch}}(f)$ can be constructed by taking the expected *total* loss for *both* observations in a random pair $(Z^{(a)}, Z^{(b)})$ when the value of X_1 is switched, and dividing by 2, which has the same expectation: $e_{\text{switch}}(f) = \frac{1}{2}\mathbb{E}[h_f(Z^{(a)}, Z^{(b)}) + h_f(Z^{(b)}, Z^{(a)})]$.

As a reference point, we compare $e_{\text{switch}}(f)$ against the standard expected loss when none of the variables are switched, $e_{\text{orig}}(f) := \mathbb{E}h_f(Z^{(a)}, Z^{(a)}) = \mathbb{E}L(f, Z)$. We define *model reliance* (MR) as the ratio of these two expected losses:

$$MR(f) := \frac{e_{\text{switch}}(f)}{e_{\text{orig}}(f)}.$$

Higher values of $MR(f)$ signify greater reliance of f on X_1 , and $MR(f) = 1$ signifies no reliance on X_1 . Although unintuitive, it is possible for a prediction model to have a MR value less than 1. However, in such cases there will often exist another prediction model with lower expected loss, and with MR precisely equal to 1 (see Section A.2 of the supplement).

Our MR measure is inspired by the tree-level, permutation-based importance measure of Random Forests (Breiman, 2001; Breiman et al., 2001). Similar estimands have more recently been proposed by Zhu et al. (2015); Gregorutti et al. (2015, 2017), for the special case when f is the conditional expectation of Y (i.e., $f(x) = \mathbb{E}(Y|X = x)$), and by Datta et al. (2016) for the purposes of studying a variable’s influence on predicted risk. We compare and contrast these approaches further in Section 4.

Model reliance could alternatively be defined as a difference rather than a ratio – i.e., with $MR_{\text{difference}}(f) := e_{\text{switch}}(f) - e_{\text{orig}}(f)$. We discuss such a definition in Section A.7 of the supplement. Many of the results in our paper remain similar under either definition.

3.1.1 Estimating model reliance with U-statistics

Given a model f and dataset $\mathbf{Z} = \begin{bmatrix} \mathbf{y} & \mathbf{X} \end{bmatrix}$, we estimate $e_{\text{orig}}(f)$ with the standard empirical loss

$$\hat{e}_{\text{orig}}(f) := \frac{1}{n} \sum_{i=1}^n L(f, \mathbf{Z}_{[i, \cdot]}) = \frac{1}{n} \sum_{i=1}^n L\{f, (\mathbf{y}_{[i]}, \mathbf{X}_{1[i, \cdot]}, \mathbf{X}_{2[i, \cdot]})\} = \hat{\mathbb{E}}L(f, Z),$$

where $\hat{\mathbb{E}}$ denotes the empirical expectation. We estimate $e_{\text{switch}}(f)$ with

$$\begin{aligned}\hat{e}_{\text{switch}}(f) &:= \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} h_f(\mathbf{Z}_{[i,\cdot]}, \mathbf{Z}_{[j,\cdot]}) \\ &= \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} L\{f, (\mathbf{y}_{[j]}, \mathbf{X}_{1[i,\cdot]}, \mathbf{X}_{2[j,\cdot]})\}.\end{aligned}\tag{3.1}$$

To illustrate the connection between Eq 3.1 and the variable importance approach of Breiman (2001), let $\{\boldsymbol{\pi}_1, \dots, \boldsymbol{\pi}_{n!}\}$ be a set of n -length vectors, each containing a different permutation of the set $\{1, \dots, n\}$. The approach of Breiman (2001) is analogous to computing the loss $\sum_{i=1}^n L\{f, (\mathbf{y}_{[i]}, \mathbf{X}_{1[\boldsymbol{\pi}_l[i,\cdot]}], \mathbf{X}_{2[i,\cdot]})\}$ for a randomly chosen permutation vector $\boldsymbol{\pi}_l \in \{\boldsymbol{\pi}_1, \dots, \boldsymbol{\pi}_{n!}\}$. Similarly, our calculation in Eq 3.1 is proportional to the sum of losses over all possible $(n!)$ permutations, excluding the n unique combinations of the rows of \mathbf{X}_1 and the rows of $\begin{bmatrix} \mathbf{X}_2 & \mathbf{y} \end{bmatrix}$ that appear in the original sample: $\sum_{l=1}^{n!} \sum_{i=1}^n L\{f, (\mathbf{y}_{[i]}, \mathbf{X}_{1[\boldsymbol{\pi}_l[i,\cdot]}], \mathbf{X}_{2[i,\cdot]})\} 1(\boldsymbol{\pi}_l[i] \neq i)$ (see Section A.3 of the supplement).

Alternatively, if the summation over all possible pairs in Eq 3.1 is computationally prohibitive due to sample size, another estimator of $e_{\text{switch}}(f)$ is

$$\hat{e}_{\text{divide}}(f) := \frac{1}{2\lfloor n/2 \rfloor} \sum_{i=1}^{\lfloor n/2 \rfloor} \{h_f(\mathbf{Z}_{[i,\cdot]}, \mathbf{Z}_{[i+\lfloor n/2 \rfloor, \cdot]}) + h_f(\mathbf{Z}_{[i+\lfloor n/2 \rfloor, \cdot]}, \mathbf{Z}_{[i,\cdot]})\}.\tag{3.2}$$

The above estimator divides the sample into a single, specific grouping of $\lfloor n/2 \rfloor$ pairs, and averages across these pairs. In this paper, we primarily use $\hat{e}_{\text{switch}}(f)$ to estimate $e_{\text{switch}}(f)$, rather than $\hat{e}_{\text{divide}}(f)$. In fact, we show that in certain cases $\hat{e}_{\text{switch}}(f)$ can be computed exactly without evaluating all possible pairings (see Section 3.1.3).

Finally, we can estimate $MR(f)$ with the plug-in estimator

$$\widehat{MR}(f) = \frac{\hat{e}_{\text{switch}}(f)}{\hat{e}_{\text{orig}}(f)},$$

which we refer to as the “empirical” model reliance of f on X_1 .

Both $\hat{e}_{\text{switch}}(f)$ and $\hat{e}_{\text{divide}}(f)$ belong to the well studied class of U-statistics. As a result, $\hat{e}_{\text{switch}}(f)$ and $\hat{e}_{\text{divide}}(f)$ are unbiased, asymptotically normal under a finite moments condition, and have finite-sample probabilistic bounds under the condition that $0 \leq L(f, (y, x_1, x_2)) \leq B_{\text{ind}}$ for any $(y, x_1, x_2) \in (\mathcal{Y} \times \mathcal{X}_1 \times \mathcal{X}_2)$, where B_{ind} is a known constant (Hoeffding, 1948; Serfling, 1980).

3.1.2 Model reliance and causal effects

A substantial portion of the statistical literature is aimed at discovering the causal effect of a treatment or exposure. It is natural to ask how such a goal may relate to our framework. Following this question, in this section we show the mathematical connection between model reliance and the causal, conditional treatment effect of a binary treatment.

For consistency with the causal inference literature, we temporarily rename the random variables (Y, X_1, X_2) as (Y, T, C) , with realizations (y, t, c) . Here, $T := X_1$ represents a binary treatment indicator, $C := X_2$ represents a set of baseline covariates, and Y represents an outcome of interest. Under this notation, $e_{\text{orig}}(f)$ represents the expected loss of a prediction function f , and $e_{\text{switch}}(f)$ denotes the expected loss in a pair of observations in which the treatment has been switched. Let $f^*(t, c) := \mathbb{E}(Y|C = c, T = t)$ be the (unknown) conditional expectation function for Y .

Let Y_1 and Y_0 be potential outcomes under treatment and control respectively, such that $Y = Y_0(1 - T) + Y_1T$. The treatment effect for an individual is defined as $Y_1 - Y_0$, and the average treatment effect is defined as $\mathbb{E}(Y_1 - Y_0)$. Let $\mathcal{TE}(c) := \mathbb{E}(Y_1 - Y_0|C = c)$ be the (unknown) conditional average treatment effect of T for all patients with $C = c$. Causal inference methods typically assume $(Y_1, Y_0) \perp T|C$ (conditional ignorability), and $0 < P(T = 1|C = c) < 1$ for all values of c (positivity), in order for f^* or \mathcal{TE} to be identifiable.

The next theorem quantifies the relation between the conditional average treatment effect function, \mathcal{TE} , and the model reliance of f^* on X_1 , as measured by $e_{\text{switch}}(f^*) - e_{\text{orig}}(f^*)$.

Theorem 1. *For any prediction model f , let $e_{\text{orig}}(f)$ and $e_{\text{switch}}(f)$ be defined based on the squared error loss $L(f, (y, t, c)) := (y - f(t, c))^2$. Under the assumption that $(Y_1, Y_0) \perp T | C$ (conditional ignorability), we have*

$$e_{\text{switch}}(f^*) - e_{\text{orig}}(f^*) = \text{Var}(T) \sum_{t \in \{0,1\}} \mathbb{E}_{C|T=t} (\mathcal{TE}(C)^2), \quad (3.3)$$

where $\text{Var}(T)$ is the marginal variance of the treatment assignment.

Intuitively, the difference between $e_{\text{switch}}(f^*)$ and $e_{\text{orig}}(f^*)$ depends on the treatment prevalence and the treatment effect for each covariate profile c . For example, if all patients are treated, then scrambling the treatment in a random pair of observations has no effect on the loss. In this case we see that $\text{Var}(T) = 0$ and $e_{\text{switch}}(f^*) = e_{\text{orig}}(f^*)$. Likewise, if the treatment effect is zero for every covariate profile c , then $\mathbb{E}_{C|T}(\mathcal{TE}(C)^2) = 0$, and $e_{\text{switch}}(f^*) = e_{\text{orig}}(f^*)$. If the treatment effect is positive and constant for all values of C , then a larger treatment effect will result in a larger value for $e_{\text{switch}}(f^*) - e_{\text{orig}}(f^*)$, and a higher reliance of f^* on T .

Importantly, $\mathbb{E}(\mathcal{TE}(C)^2)$ will yield different conclusions than the average treatment effect $\mathbb{E}(\mathcal{TE}(C))$ when there is treatment effect heterogeneity (i.e., when $\text{Var}(\mathcal{TE}(C)) = \mathbb{E}(\mathcal{TE}(C)^2) - \mathbb{E}(\mathcal{TE}(C))^2 > 0$). For example, if a treatment is harmful in one subpopulation, but helpful in another, then the average treatment effect may be zero while the average of the squared conditional treatment effect will be positive.

3.1.3 Model reliance for linear models and additive models

For linear models and the squared error loss, we can show both an interpretable definition of model reliance, as measured by $e_{\text{switch}}(f) - e_{\text{orig}}(f)$, as well as a computationally efficient formula for $\hat{e}_{\text{switch}}(f)$. The result is similar to Theorem 1, and augments results from Gregorutti et al. (2017).

Theorem 2. *For any prediction model f , let $e_{\text{orig}}(f)$, $e_{\text{switch}}(f)$, $\hat{e}_{\text{orig}}(f)$, and $\hat{e}_{\text{switch}}(f)$ be defined based on the squared error loss $L(f, (y, x_1, x_2)) := (y - f(x_1, x_2))^2$ for $y \in \mathbb{R}$, $x_1 \in \mathbb{R}^{p_1}$,*

and $x_2 \in \mathbb{R}^{p_2}$, where p_1 and p_2 are positive integers. Let $\beta = (\beta_1, \beta_2)$ and f_β satisfy $\beta_1 \in \mathbb{R}^{p_1}$, $\beta_2 \in \mathbb{R}^{p_2}$, and $f_\beta(x) = x'\beta = X_1'\beta_1 + X_2'\beta_2$. Then

$$e_{\text{switch}}(f_\beta) - e_{\text{orig}}(f_\beta) = 2\text{Cov}(Y, X_1)\beta_1 - 2\beta_2'\text{Cov}(X_2, X_1)\beta_1, \quad (3.4)$$

and, for finite samples,

$$\hat{e}_{\text{switch}}(f_\beta) = \frac{1}{n} \left\{ \mathbf{y}'\mathbf{y} - 2 \begin{bmatrix} \mathbf{X}_1'\mathbf{W}\mathbf{y} \\ \mathbf{X}_2'\mathbf{y} \end{bmatrix}' \beta + \beta' \begin{bmatrix} \mathbf{X}_1'\mathbf{X}_1 & \mathbf{X}_1'\mathbf{W}\mathbf{X}_2 \\ \mathbf{X}_2'\mathbf{W}\mathbf{X}_1 & \mathbf{X}_2'\mathbf{X}_2 \end{bmatrix} \beta \right\}, \quad (3.5)$$

where $\mathbf{W} := \frac{1}{n-1}(\mathbf{1}_n\mathbf{1}_n' - \mathbf{I}_n)$, $\mathbf{1}_n$ is the n -length vector of ones, and \mathbf{I}_n is the $n \times n$ identity matrix.

Eq 3.4 shows that model reliance for linear models, as measured by $e_{\text{switch}}(f_\beta) - e_{\text{orig}}(f_\beta)$, can be interpreted in terms of the population covariances and the model coefficients. Gregorutti et al. (2017) show an equivalent formulation of Eq 3.4 under the stronger assumptions that f_β is equal to the conditional expectation function of Y (i.e., $f_\beta(x) = \mathbb{E}(Y|X = x)$), and the covariates X_1 and X_2 are centered.

Although the number of terms in the definition of $\hat{e}_{\text{switch}}(f)$ grows quadratically in n (see Eq 3.1), in the case of linear models we see from Eq 3.5 that the computational complexity of $\hat{e}_{\text{switch}}(f)$ grows *only linearly* in n . Specifically, the terms $\mathbf{X}_1'\mathbf{W}\mathbf{y}$ and $\mathbf{X}_1'\mathbf{W}\mathbf{X}_2$ in Eq 3.5 can be computed as $\frac{1}{n-1} \{(\mathbf{X}_1'\mathbf{1}_n)(\mathbf{1}_n'\mathbf{y}) - (\mathbf{X}_1'\mathbf{y})\}$ and $\frac{1}{n-1} \{(\mathbf{X}_1'\mathbf{1}_n)(\mathbf{1}_n'\mathbf{X}_2) - (\mathbf{X}_1'\mathbf{X}_2)\}$ respectively, where the computational complexity each term in parentheses grows linearly in n .

As in Gregorutti et al. (2017), both results in Theorem 2 readily generalize to additive models of the form $f_{g_1, g_2}(X_1, X_2) := g_1(X_1) + g_2(X_2)$, since permuting X_1 is equivalent to permuting $g_1(X_1)$:

$$e_{\text{switch}}(f_{g_1, g_2}) - e_{\text{orig}}(f_{g_1, g_2}) = 2\text{Cov}\{Y, g_1(X_1)\} - 2\text{Cov}\{g_2(X_2), g_1(X_1)\}.$$

3.2 Algorithm reliance

A common variable importance procedure is to run a model-fitting algorithm twice, first on all of the data, and then again after removing X_1 from the dataset. The losses for the two resulting models are then compared to determine the importance, or “necessity,” of X_1 (Gevrey et al., 2003). Because this measure is a function of two prediction models rather than one, it does not measure how much either individual model relies on X_1 . Instead, it measures *algorithm* reliance (AR) on X_1 , as the model-fitting algorithm is the common attribute between the two models.

The AR approach bears a resemblance to a likelihood ratio test statistic (Casella and Berger, 2002). A related procedure was also proposed by Breiman et al. (2001); Breiman (2001), in which the change in accuracy is observed after removing X_2 and retraining the algorithm. This procedure measures the sufficiency of X_1 for a model-fitting algorithm, or, equivalently, the necessity of X_2 .

For many model-fitting algorithms, the procedure of fully removing X_1 is reasonable and well defined. However, algorithms that require a certain number of predictor variables as input may not be well defined after X_1 has been removed; for instance, a decision tree cannot split on a missing variable. With this in mind, we propose a similar, permutation-based algorithm reliance measure in Section A.4 of the supplement.

3.3 Model class reliance

Like many statistical procedures, our MR measure (Section 3.1) produces a description of a *single* predictive model. Given a model with high predictive accuracy, MR describes how much the model’s performance hinges on covariates of interest (X_1). However, even if the best-in-class model $f^* = \arg \min_{f \in \mathcal{F}} e_{\text{orig}}(f)$ can be determined and described, there will often be many other models that perform similarly well, and that rely on X_1 to different degrees. With this notion in mind, we now study how much *any* well-performing model from a prespecified class \mathcal{F} may rely on covariates of interest.

For $\epsilon \geq 0$, let $\mathcal{R}(\epsilon, f^*, \mathcal{F}) := \{f \in \mathcal{F} : e_{\text{orig}}(f) \leq e_{\text{orig}}(f^*) + \epsilon\}$ be the subset of models with expected loss no more than ϵ above the best-in-class model f^* (see Figure 1). We refer to $\mathcal{R}(\epsilon, f^*, \mathcal{F})$ as a population-level ‘‘Rashomon set’’ around f^* . This set can be thought of as representing models that might be arrived at due to differences in data measurement, processing, filtering, model parameterization, covariate selection, or other analysis choices. We define Model Class Reliance (MCR) by maximizing and minimizing MR over $\mathcal{R}(\epsilon, f^*, \mathcal{F})$:

$$MCR_+(\epsilon, f^*, \mathcal{F}) := \max_{f \in \mathcal{R}(\epsilon, f^*, \mathcal{F})} MR(f), \quad \text{and} \quad MCR_-(\epsilon, f^*, \mathcal{F}) := \min_{f \in \mathcal{R}(\epsilon, f^*, \mathcal{F})} MR(f). \quad (3.6)$$

We assume throughout that \mathcal{F} is fixed and prespecified, and so we typically omit the notation \mathcal{F} when referring to Rashomon sets and MCR.

If $MCR_+(\epsilon, f^*)$ is low, then no well performing model exists that places high importance on X_1 , and X_1 can be discarded at low cost regardless of future modeling decisions. If $MCR_-(\epsilon, f^*)$ is large, then every well performing model must rely substantially on X_1 , and X_1 should be given careful attention during the modeling process. Here, \mathcal{F} may itself consist of several parametric model forms (e.g., all linear models and all decision tree models with less than 6 single-split nodes). We stress that the range $(MCR_-(\epsilon, f^*), MCR_+(\epsilon, f^*))$ does not depend on the *algorithm* used to select a model $f \in \mathcal{F}$. The range is valid for any algorithm producing models in \mathcal{F} , and applies for any $f \in \mathcal{F}$.

In practice, because the best-in-class model f^* is unknown, we approximate $\mathcal{R}(\epsilon, f^*)$ by replacing f^* with a known model \hat{f} that is thought to have expected loss close to that of f^* . We then estimate $MCR_-(\epsilon, \hat{f})$ and $MCR_+(\epsilon, \hat{f})$, the minimum and maximum MR values across models in $\mathcal{R}(\epsilon, \hat{f})$. This approximation is conservative in the sense that $\mathcal{R}(\epsilon, f^*) \subset \mathcal{R}(\epsilon, \hat{f})$ by the definition of f^* , and so $MCR_-(\epsilon, \hat{f}) \leq MCR_-(\epsilon, f^*)$ and $MCR_+(\epsilon, \hat{f}) \geq MCR_+(\epsilon, f^*)$ (see Figure 1). While \hat{f} can be selected by minimizing the in-sample loss, the theoretical study of $\mathcal{R}(\epsilon, \hat{f})$ is simplified under the assumption that \hat{f} is prespecified – either determined from the literature or selected using a separate dataset.

Alternatively, if an established benchmark model f_{ref} from the literature is of interest, we

can similarly estimate $MCR_-(\epsilon, f_{\text{ref}})$ and $MCR_+(\epsilon, f_{\text{ref}})$. For example, the model f_{ref} may come from a flowchart used to predict injury severity in a hospital’s emergency room, or from another quantitative decision rule that is currently implemented in practice. Because the same estimation techniques apply without loss of generality, in the remainder of this paper we consider the problem of estimating $MCR_-(\epsilon, f_{\text{ref}})$ and $MCR_+(\epsilon, f_{\text{ref}})$ for a prespecified benchmark function $f_{\text{ref}} \in \mathcal{F}$.

To study MCR empirically, we introduce the sample analogues

$$\widehat{MCR}_+(\epsilon, f_{\text{ref}}, \mathcal{F}) := \max_{f \in \hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F})} \widehat{MR}(f) \quad \text{and} \quad \widehat{MCR}_-(\epsilon, f_{\text{ref}}, \mathcal{F}) := \min_{f \in \hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F})} \widehat{MR}(f), \quad (3.7)$$

where $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}) := \{f \in \mathcal{F} : \hat{e}_{\text{orig}}(f) \leq \hat{e}_{\text{orig}}(f_{\text{ref}}) + \epsilon\}$. Hereafter, because we assume that the model class \mathcal{F} and benchmark function f_{ref} plugged into Eqs 3.6 & 3.7 are fixed, we typically omit them in notation. We refer to $\widehat{MCR}_+(\epsilon)$ and $\widehat{MCR}_-(\epsilon)$ as “empirical” MCR measures, and to $\hat{\mathcal{R}}(\epsilon)$ as an “empirical Rashomon set.” We give an example to illustrate these empirical measures in Section 5.

In Section C.10 of the supplement we consider an alternate formulation of Rashomon sets and MCR where we replace the relative loss threshold in the definition of $\mathcal{R}(\epsilon)$ with an absolute loss threshold. This alternate formulation can be similar in practice, but still requires the specification of a reference function to ensure that $\mathcal{R}(\epsilon)$ and $\hat{\mathcal{R}}(\epsilon)$ are nonempty.

3.3.1 Finite-sample bounds for model class reliance

In this section we derive finite-sample, probabilistic bounds for $MCR_+(\epsilon)$ and $MCR_-(\epsilon)$ based on empirical model class reliance. While the bounds we present are conservative, they imply that, under minimal assumptions, $\widehat{MCR}_+(\epsilon)$ and $\widehat{MCR}_-(\epsilon)$ are sensible proxies for $MCR_+(\epsilon)$ and $MCR_-(\epsilon)$. Thus, in Sections 5 and 6, we focus our attention on $\widehat{MCR}_+(\epsilon)$ and $\widehat{MCR}_-(\epsilon)$.

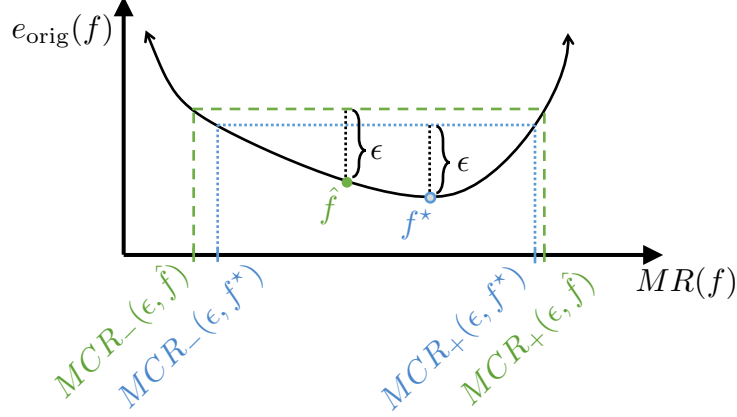


Figure 1: Nested Rashomon sets for f^* and \hat{f} – Above we show the relationship between model reliance (x-axis) and expected loss (y-axis) for a hypothetical model class \mathcal{F} . We mark the best-in-class model f^* by the blue and gray point. We mark the model \hat{f} by the green point. For each possible model reliance value $r \geq 0$, the curved black line shows the lowest possible expected loss for a function in $f \in \mathcal{F}$ satisfying $MR(f) = r$. The set $\mathcal{R}(\epsilon, f^*)$ contains all models in \mathcal{F} within the blue dotted lines, above, and the set $\mathcal{R}(\epsilon, \hat{f})$ contains all models in \mathcal{F} within the green dashed lines. Along the x-axis, we mark the smallest and largest MR values within each Rashomon set. We see that $\mathcal{R}(\epsilon, f^*) \subset \mathcal{R}(\epsilon, \hat{f})$, which implies that $MCR_-(\epsilon, \hat{f}) \leq MCR_-(\epsilon, f^*)$ and $MCR_+(\epsilon, \hat{f}) \geq MCR_-(\epsilon, f^*)$.

To derive these results we introduce three bounded loss assumptions, each of which can be assessed empirically. Let $b_{\text{avg}}, B_{\text{ind}}, B_{\text{ref}}, B_{\text{avg}} \in \mathbb{R}$ be known constants.

Assumption 3. (*Bounded individual loss*) For a given model $f \in \mathcal{F}$, assume that $0 \leq L(f, (y, x_1, x_2)) \leq B_{\text{ind}}$ for any $(y, x_1, x_2) \in (\mathcal{Y} \times \mathcal{X}_1 \times \mathcal{X}_2)$.

Assumption 4. (*Bounded relative loss*) For a given model $f \in \mathcal{F}$, assume that $|L(f, (y, x_1, x_2)) - L(f_{\text{ref}}, (y, x_1, x_2))| \leq B_{\text{ref}}$ for any $(y, x_1, x_2) \in \mathcal{Z}$.

Assumption 5. (*Bounded average loss*) For a given model $f \in \mathcal{F}$, assume that $\mathbb{P}\{0 < b_{\text{avg}} \leq \hat{e}_{\text{orig}}(f) \leq B_{\text{avg}}\} = 1$.

Each assumption is a property of a specific model $f \in \mathcal{F}$. The notation B_{ind} and B_{ref} refer to bounds for any individual observation, and the notation b_{avg} and B_{avg} refer to bounds on the average loss L in a sample.

We give example methods of determining B_{ind} in Sections B.4.2 & B.5.2 of the supplement.

For Assumption 5, we can approximate b_{avg} by training a highly flexible model to the data, and setting b_{avg} equal to half (or any positive fraction) of the resulting cross-validated loss. To determine B_{avg} we can simply set $B_{\text{avg}} = B_{\text{ind}}$, although this may be conservative if observations with similar or identical covariate profiles have different outcomes. For example, in the case of binary classification models for non-separated groups (see Section 5), no linear classifier can misclassify all observations, and so it must hold that $B_{\text{ind}} > B_{\text{avg}}$. Similarly, if f_{ref} satisfies Assumption 3, then B_{ref} may be conservatively set equal to B_{ind} .

If model reliance is redefined as a difference rather than a ratio, then a similar form of the results in this section will apply without Assumption 5 (see Section A.7 of the supplement). A similar form of the results in this section will also hold if we define the Rashomon set in terms of an absolute loss threshold (see Section C.10 of the supplement).

Based on the above assumptions, we can create a finite-sample upper bound for $MCR_+(\epsilon)$ and lower bound for $MCR_-(\epsilon)$.

Theorem 6. *Given a constant $\epsilon \in \mathbb{R}$, let $f_{+,\epsilon} \in \arg \max_{\mathcal{R}(\epsilon)} MR(f)$ and $f_{-,\epsilon} \in \arg \min_{\mathcal{R}(\epsilon)} MR(f)$ be prediction models that attain the highest and lowest model reliance among models in $\mathcal{R}(\epsilon)$. If $f_{+,\epsilon}$ and $f_{-,\epsilon}$ satisfy Assumptions 3, 4 & 5, then*

$$\mathbb{P} \left(MCR_+(\epsilon) > \widehat{MCR}_+(\epsilon_1) + \mathcal{Q}_1 \right) \leq \delta, \quad (3.8)$$

and

$$\mathbb{P} \left(MCR_-(\epsilon) < \widehat{MCR}_-(\epsilon_1) - \mathcal{Q}_1 \right) \leq \delta, \quad (3.9)$$

where $\epsilon_1 := \epsilon + 2B_{\text{ref}}\sqrt{\frac{\log(3\delta^{-1})}{2n}}$, and $\mathcal{Q}_1 := \frac{B_{\text{avg}}}{b_{\text{avg}}} - \frac{B_{\text{avg}} - B_{\text{ind}}\sqrt{\frac{\log(6\delta^{-1})}{n}}}{b_{\text{avg}} + B_{\text{ind}}\sqrt{\frac{\log(6\delta^{-1})}{2n}}}$.

Eq 3.8 states that, with high probability, $MCR_+(\epsilon)$ is no higher than $\widehat{MCR}_+(\epsilon_1)$ added to a shrinking error term \mathcal{Q}_1 , where ϵ_1 approaches ϵ as n increases. A similar interpretation holds for Eq 3.9. We provide a visualization of the result in Section A.5 of the supplement, and also give a brief sketch of the proof here. First, we enlarge the empirical Rashomon set by increasing ϵ to ϵ_1 , such that, by Hoeffding's inequality, $f_{+,\epsilon} \in \hat{\mathcal{R}}(\epsilon_1)$ with high probability. When

$f_{+, \epsilon} \in \hat{\mathcal{R}}(\epsilon_1)$, we know that $\widehat{MR}(f_{+, \epsilon}) \leq \widehat{MCR}_+(\epsilon_1)$ by the definition of $\widehat{MCR}_+(\epsilon_1)$. Next, the term \mathcal{Q}_1 accounts for estimator error of $\widehat{MR}(f_{+, \epsilon})$ relative to $MR(f_{+, \epsilon}) = MCR_+(\epsilon)$. Thus, we can relate $\widehat{MR}(f_{+, \epsilon})$ to both $\widehat{MCR}_+(\epsilon_1)$ and $MCR_+(\epsilon)$ in order to obtain Eq 3.8. Similar steps can be applied to obtain Eq 3.9.

The bounds in Theorem 6 naturally account for potential overfitting without an explicit limit on model class complexity, such as a covering number (Bousquet et al., 2004; Rudin and Schapire, 2009). Instead, these bounds depend on being able to fully optimize MR across sets in the form of $\hat{\mathcal{R}}(\epsilon)$. If we allow our model class \mathcal{F} to become more flexible, then the size of $\hat{\mathcal{R}}(\epsilon)$ will also increase. Because the bounds in Theorem 6 result from optimizing over $\hat{\mathcal{R}}(\epsilon)$, increasing the size of $\hat{\mathcal{R}}(\epsilon)$ results in wider, more conservative bounds. In this way, Eqs 3.8 and 3.9 implicitly capture model class complexity.

A corollary of Theorem 6 is that we can create a probabilistic bound for the reliance of the (unknown) best-in-class model f^* on X_1 .

Corollary 7. *Let $f^* \in \arg \min_{f \in \mathcal{F}} e_{orig}(f)$ be a prediction model that attains the lowest possible expected loss, and let $f_{+, \epsilon}$ and $f_{-, \epsilon}$ be defined as in Theorem 6. If $f_{+, \epsilon}$ and $f_{-, \epsilon}$ satisfy Assumptions 3, 4 and 5, then*

$$\mathbb{P} \left(MR(f^*) \in \left[\widehat{MCR}_-(\epsilon_2) - \mathcal{Q}_2, \quad \widehat{MCR}_+(\epsilon_2) + \mathcal{Q}_2 \right] \right) \geq 1 - \delta,$$

$$\text{where } \epsilon_2 := 2B_{ref} \sqrt{\frac{\log(6\delta^{-1})}{2n}}, \text{ and } \mathcal{Q}_2 := \frac{B_{avg}}{b_{avg}} - \frac{B_{avg} - B_{ind}}{b_{avg} + B_{ind}} \sqrt{\frac{\log(12\delta^{-1})}{2n}}.$$

The above result does not require that f^* be unique. If several models achieve the minimum possible expected loss, the above boundaries apply simultaneously for each of them. In the special case when the true conditional expectation function $\mathbb{E}(Y|X_1, X_2)$ is equal to f^* , then we have a boundary for the reliance of the function $\mathbb{E}(Y|X_1, X_2)$ on X_1 . This reliance bound can also be translated into a causal statement using Theorem 1.

So far, Theorem 6 allows us to cap the range of MR values corresponding to models that predict well, but it does not necessarily provide a complete understanding when this range is

large. For example, even if the lower bound on $MCR_-(\epsilon)$ from Eq 3.9 is below 1, we are not able to conclude that there exists a well-performing model $f_0 \in \mathcal{R}(\epsilon)$ with no reliance on X_1 (i.e., with $MR(f_0) = 1$). To conclude that such a model exists, we need an upper bound on $MCR_-(\epsilon)$. Likewise, in order to make conclusions regarding the existence of well-performing models with high reliance on X_1 , we need a lower bound on $MCR_+(\epsilon)$.

To create such bounds, we take a contrary approach to that of Theorem 6, where we had expanded the empirical Rashomon set by increasing ϵ to ϵ_1 . We now contract the empirical Rashomon set by subtracting a buffer term from ϵ . This requires that we generalize the definition of an empirical Rashomon set to $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}) := \{f_{\text{ref}}\} \cup \{f \in \mathcal{F} : \hat{e}_{\text{orig}}(f) \leq \hat{e}_{\text{orig}}(f_{\text{ref}}) + \epsilon\}$ for $\epsilon \in \mathbb{R}$. The definition is unchanged for $\epsilon \geq 0$, but for $\epsilon < 0$ the explicit inclusion of f_{ref} now ensures that $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F})$ is nonempty. As before, we typically omit the notation f_{ref} and \mathcal{F} , writing $\hat{\mathcal{R}}(\epsilon)$ instead.

Creating these additional boundaries will also require a limit on the complexity of \mathcal{F} . We propose a complexity measure in the form of a covering number. Specifically, we define the set of functions \mathcal{G}_r as an r -margin-expectation-cover if for any $f \in \mathcal{F}$ and any distribution D , there exists $g \in \mathcal{G}_r$ such that

$$\mathbb{E}_{Z \sim D} |L(f, Z) - L(g, Z)| \leq r. \quad (3.10)$$

We define the *covering number* $\mathcal{N}(\mathcal{F}, r)$ to be the size of the smallest r -margin-expectation-cover for \mathcal{F} . We compare $\mathcal{N}(\mathcal{F}, r)$ to related measures of model class complexity in Section A.6 of the supplement. In general, we use $\mathbb{P}_{V \sim D}$ and $\mathbb{E}_{V \sim D}$ to denote probabilities and expectations with respect to a random variable V following the distribution D . We abbreviate these quantities as \mathbb{P}_V and \mathbb{E}_V respectively when D is clear from context, or as \mathbb{P}_D and \mathbb{E}_D respectively when V is clear from context. Unless otherwise stated, all expectations and probabilities are taken with respect to the (unknown) population distribution.

Equipped with this complexity measure, we can determine a probabilistic lower bound for $MCR_+(\epsilon)$, and upper bound for $MCR_-(\epsilon)$.

Theorem 8. *Given constants $\epsilon \geq 0$ and $r > 0$, if Assumptions 3, 4 and 5 hold for all $f \in \mathcal{F}$, and then*

$$\mathbb{P} \left(MCR_+(\epsilon) < \widehat{MCR}_+(\epsilon_3) - \mathcal{Q}_3 \right) \leq \delta, \quad (3.11)$$

and

$$\mathbb{P} \left(MCR_-(\epsilon) > \widehat{MCR}_-(\epsilon_3) + \mathcal{Q}_3 \right) \leq \delta, \quad (3.12)$$

where $\epsilon_3 := \epsilon - 2B_{\text{ref}}\sqrt{\frac{\log(4\delta^{-1}\mathcal{N}(\mathcal{F}, r))}{2n}} - 2r$, and

$$\mathcal{Q}_3 := \frac{B_{\text{avg}}}{b_{\text{avg}}} - \frac{B_{\text{avg}} - \left\{ B_{\text{ind}}\sqrt{\frac{\log(8\delta^{-1}\mathcal{N}(\mathcal{F}, r\sqrt{2}))}{n}} + 2r\sqrt{2} \right\}}{b_{\text{avg}} + \left\{ B_{\text{ind}}\sqrt{\frac{\log(8\delta^{-1}\mathcal{N}(\mathcal{F}, r))}{2n}} + 2r \right\}}.$$

Eq 3.12 states that, with high probability, $MCR_-(\epsilon)$ is no higher than $\widehat{MCR}_-(\epsilon_3)$ added to an error term \mathcal{Q}_3 , where \mathcal{Q}_3 and $(\epsilon_3 - \epsilon)$ can be made arbitrarily small by shrinking r and increasing n . A similar interpretation holds for the upper bound on $MCR_+(\epsilon)$ in Eq 3.11. We provide a visualization of this result in Section A.5 of the supplement.

In some cases, it may be possible to improve the bounds in Theorem 8 by splitting the sample into two parts, using the first split to intelligently select a subset $\mathcal{F}_s \subset \mathcal{F}$, and using the second split to calculate boundaries. For any subset $\mathcal{F}_s \subset \mathcal{F}$, the value of $MCR_+(\epsilon, f_{\text{ref}}, \mathcal{F}_s)$ will naturally serve as a lower bound on $MCR_+(\epsilon, f_{\text{ref}}, \mathcal{F})$. Thus, rather than using Eq 3.11 to lower bound $MCR_+(\epsilon, f_{\text{ref}}, \mathcal{F})$ directly, we can search for a simpler model class \mathcal{F}_s such that $MCR_+(\epsilon, f_{\text{ref}}, \mathcal{F}_s) \approx MCR_+(\epsilon, f_{\text{ref}}, \mathcal{F})$, and $\mathcal{N}(\mathcal{F}_s, r) \ll \mathcal{N}(\mathcal{F}, r)$. Balancing these two criteria may lead to a tighter bound from Theorem 8. For example, consider the special case where $\mathcal{F} = \{f_{\boldsymbol{\theta}} : \boldsymbol{\theta} \in \mathbb{R}^d\}$ is indexed by a real-valued parameter $\boldsymbol{\theta}$. Given a training dataset, let $\boldsymbol{\theta}_{\text{orig}} \in \arg \min_{\boldsymbol{\theta} \in \mathbb{R}^d} \hat{e}_{\text{orig}}(f_{\boldsymbol{\theta}})$ and let $\boldsymbol{\theta}_+ \in \arg \max_{\{\boldsymbol{\theta} : f_{\boldsymbol{\theta}} \in \hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F})\}} \widehat{MR}(f_{\boldsymbol{\theta}})$, where $\hat{e}_{\text{orig}}(f_{\boldsymbol{\theta}})$ and $\widehat{MR}(f_{\boldsymbol{\theta}})$ are computed using training data. We can then set \mathcal{F}_s as the subset of models

resulting from convex combinations of $\boldsymbol{\theta}_{\text{orig}}$ and $\boldsymbol{\theta}_+$:

$$\mathcal{F}_s = \{f_{\boldsymbol{\theta}} \in \mathcal{F} : \boldsymbol{\theta} = w\boldsymbol{\theta}_{\text{orig}} + (1-w)\boldsymbol{\theta}_+; w \in [0, 1]\}. \quad (3.13)$$

The bound from Eq 3.11 can be evaluated for \mathcal{F}_s in a held-out dataset, potentially resulting in a tighter bound for $MCR_+(\epsilon, f_{\text{ref}}, \mathcal{F})$. In the case of linear classifiers, we can analytically derive a covering number for \mathcal{F}_s .

Proposition 9. *Consider the classification setting where $\mathcal{X} = \mathbb{R}^p$; $\mathcal{Y} = \{-1, 1\}$; L is the hinge loss $L(f, (y, x)) = (\delta - yf(x))_+$ for $\delta \in \mathbb{R}$; \mathcal{F} is the set of linear classifiers $\{f_{\boldsymbol{\theta}} : f_{\boldsymbol{\theta}}(x) = x'\boldsymbol{\theta}; \boldsymbol{\theta} \in \mathbb{R}^p\}$; and \mathcal{F}_s is defined as in Eq 3.13 for the prespecified vectors $\boldsymbol{\theta}_{\text{orig}}, \boldsymbol{\theta}_+ \in \mathbb{R}^p$. In this setting, if $|f_{\boldsymbol{\theta}_+}(x_1, x_2) - f_{\boldsymbol{\theta}_{\text{orig}}}(x_1, x_2)| \leq c$ for all $(x_1, x_2) \in (\mathcal{X}_1 \times \mathcal{X}_2)$, then $\mathcal{N}(\mathcal{F}_s, r) \leq \left\lceil \frac{c}{2r} \right\rceil$ holds for any $r \in \mathbb{R}$.*

Intuitively, Proposition 9 states that if the parameter vectors $\boldsymbol{\theta}_+$ and $\boldsymbol{\theta}_{\text{orig}}$ produce similar predictions, then there exists a bound on the size of the r -margin-expectation-cover for the model class formed by convex combinations of $\boldsymbol{\theta}_+$ and $\boldsymbol{\theta}_{\text{orig}}$ (as in Eq 3.13).

3.3.2 General purpose, finite-sample CIs from Rashomon sets

Corollary 7 shows that Rashomon sets can be used to derive confidence intervals (CIs) for the MR of best-in-class model(s). A similar approach can be used to create finite-sample CIs for other summary descriptions of best-in-class model(s).

To illustrate this approach, let $\phi : \mathcal{F} \rightarrow \mathbb{R}$ be a descriptor of interest for models in \mathcal{F} . For example, if $f_{\boldsymbol{\beta}}$ is the linear model $f_{\boldsymbol{\beta}}(x) = x'\boldsymbol{\beta}$, then ϕ may be defined as the norm of the associated coefficient vector (i.e., $\phi(f_{\boldsymbol{\beta}}) = \|\boldsymbol{\beta}\|_2^2$) or the prediction $f_{\boldsymbol{\beta}}$ would assign given a specific set of covariates x_{new} (i.e., $\phi(f_{\boldsymbol{\beta}}) = f_{\boldsymbol{\beta}}(x_{\text{new}})$). For simplicity, we assume that $\phi(f)$ can be determined exactly for any model $f \in \mathcal{F}$. Note that this condition is not satisfied if we choose model reliance as our descriptor ϕ , and so, because of this simplification, the results of this section do not fully replace those of Section 3.3.1. We also temporarily assume

that the best-in-class model $f^* \in \mathcal{F}$ *uniquely* minimizes the expected loss. In this setting, the following proposition allows us to create finite-sample CIs for $\phi(f^*)$ based on empirical Rashomon sets.

Proposition 10. *Let $\hat{a}_-(\epsilon_4) := \min_{f \in \hat{\mathcal{R}}(\epsilon_4)} \phi(f)$ and $\hat{a}_+(\epsilon_4) := \max_{f \in \hat{\mathcal{R}}(\epsilon_4)} \phi(f)$, where $\epsilon_4 := 2B_{\text{ref}}\sqrt{\frac{\log(\delta^{-1})}{2n}}$. Let $f^* \in \arg \min_{f \in \mathcal{F}} e_{\text{orig}}(f)$ be the prediction model that uniquely attains the lowest possible expected loss. If f^* satisfies Assumption 4, then*

$$\mathbb{P}\{\phi(f^*) \in [\hat{a}_-(\epsilon_4), \hat{a}_+(\epsilon_4)]\} \geq 1 - \delta.$$

Proposition 10 generates the finite-sample CI $[\hat{a}_-(\epsilon_4), \hat{a}_+(\epsilon_4)]$, which can be interpreted as the range of values $\phi(f)$ corresponding to models f with empirical loss not substantially above that of f_{ref} . Thus, the interval has both a rigorous coverage rate and a coherent in-sample interpretation. This in-sample interpretation is explored further by Coker et al. (2018)¹, who also discuss connections between profile likelihood intervals and sets of models with strong in-sample accuracy. The proof of Proposition 10 uses Hoeffding’s inequality to show that f^* is contained in $\hat{\mathcal{R}}(\epsilon_4)$ with high probability. Our assumption that f^* uniquely minimizes $e_{\text{orig}}(f)$ over $f \in \mathcal{F}$ can be removed if we consider the following version of Proposition 10:

Proposition 11. *Let $\hat{a}_-(\epsilon_5) := \min_{f \in \hat{\mathcal{R}}(\epsilon_5)} \phi(f)$ and $\hat{a}_+(\epsilon_5) := \max_{f \in \hat{\mathcal{R}}(\epsilon_5)} \phi(f)$, where $\epsilon_5 := 2B_{\text{ref}}\sqrt{\frac{\log(2\delta^{-1})}{2n}}$. If Assumption 4 holds for all $f \in \mathcal{R}(0)$, then*

$$\mathbb{P}[\{\phi(f) : f \in \mathcal{R}(0)\} \subset [\hat{a}_-(\epsilon_5), \hat{a}_+(\epsilon_5)]] \geq 1 - \delta.$$

In contrast to Proposition 10, Proposition 11 creates a finite-sample CI *for the range* of values $\phi(f)$ corresponding to the models with expected loss no greater than f_{ref} . By definition,

¹This paper is concurrent work.

this range includes $\phi(f^*)$ for any f^* minimizing the expected loss. Applying Propositions 10 & 11 allows us to reframe a wide set of statistical inference problems as in-sample optimization problems.

3.3.3 Calculating empirical model class reliance

In Section B of the supplement, we propose a binary search procedure to bound the values of $\widehat{MCR}_-(\epsilon)$ and $\widehat{MCR}_+(\epsilon)$ (see Eq 3.7), where each step of the search consists of minimizing a linear combination of $\hat{e}_{\text{orig}}(f)$ and $\hat{e}_{\text{switch}}(f)$ across $f \in \mathcal{F}$. Our approach is related to the fractional programming approach of Dinkelbach (1967), but accounts for the fact that the problem is constrained by the value of the denominator, $\hat{e}_{\text{orig}}(f)$. We additionally show that, for many model classes, computing $\widehat{MCR}_-(\epsilon)$ only requires that we minimize *convex* combinations of $\hat{e}_{\text{orig}}(f)$ and $\hat{e}_{\text{switch}}(f)$, which is no more difficult than minimizing the average loss over an expanded and reweighted sample.

Computing $\widehat{MCR}_+(\epsilon)$ however will require that we are able to minimize arbitrary linear combinations of $\hat{e}_{\text{orig}}(f)$ and $\hat{e}_{\text{switch}}(f)$. Thus, in Sections B.3, B.4, & B.5 of the supplement, we show specifically how to minimize arbitrary linear combinations of $\hat{e}_{\text{orig}}(f)$ and $\hat{e}_{\text{switch}}(f)$ when \mathcal{F} is the class of linear models, regularized linear models, or linear models in a reproducing kernel Hilbert space (RKHS). Even when the associated objective functions are non-convex, we can tractably obtain global minima for these model classes. We also discuss procedures to determine an upper bound B_{ind} on the loss for any observation when using these model classes.

3.4 Model reliance on imputation residuals of correlated predictors

One common scenario where multiple models achieve low loss is when the sets of predictors X_1 and X_2 are highly correlated, or contain redundant information. Models may predict well either through reliance on X_1 , or through reliance on X_2 , and so MCR will correctly identify a wide range of potential reliances on X_1 . However, we may specifically be interested in the

information in X_1 that is not redundant with information in X_2 . In other words, we may wish to know how much models that fully exhaust the information in X_2 can additionally rely on the information in X_1 .

For example, age and accumulated wealth may be correlated, and both may be predictive of future promotion. We may wish to know the potential importance of wealth when predicting promotions, but only for models that fully incorporate age.

To achieve this, we propose a preprocessing step in which the variables of interest (X_1) are imputed from the remaining variables, and a second step where model class reliance for the imputation residual is studied. Let $g_{\text{impute}} : \mathcal{X}_2 \rightarrow \mathcal{X}_1$ be a prespecified model to impute X_1 from X_2 , let $\tilde{X}_1 := X_1 - g_{\text{impute}}(X_2)$, and let \mathcal{F} be a prespecified class of models that use \tilde{X}_1 and X_2 to predict Y . After computing \tilde{X}_1 , we can estimate the model class reliance of \mathcal{F} on \tilde{X}_1 . Such an approach will generally result in a smaller value of $MCR_+(\epsilon)$ relative to the result that would occur from proceeding without an imputation preprocessing step.

4 Related work

Several common approaches for variable selection, or for describing relationships between variables, do not necessarily capture a variable’s importance. Null hypothesis testing methods can be used to investigate whether there exists a relationship between two variables. But, if such a relationship exists, they do not describe the strength of that relationship. Similarly, checking whether a variable is included by a sparse model-fitting algorithm, such as the Lasso (Hastie et al., 2009), does not describe the extent to which the variable is relied on, or could be relied on, for prediction accuracy. Partial dependence plots form a useful visualization of a prediction model’s behavior (Breiman et al., 2001; Hastie et al., 2009), but they can be difficult to interpret if multiple variables are of interest, or if the prediction model contains interaction effects. For example, consider the following model that predicts a binary outcome from two binary inputs: $f(x_1, x_2) = 1(x_1 \neq x_2)$, where 1 denotes the indicator function. This

model can produce flat partial dependence plots for both input variables, even if both inputs crucially contribute to the model’s performance.

Other methods that target variable importance are often only well-defined for models within a specific class. For example, in linear models, importance can be interpreted as the size of the (standardized) coefficient for a variable (Breiman et al., 2001; Gevrey et al., 2003). For neural networks, Garson (1991) propose a VI measure based on the weights connecting network nodes. For Random Forests (RFs), Breiman (2001); Breiman et al. (2001) propose to check the decrease in out-of-bag performance of each tree when the variable of interest is permuted, and to average this value across trees in the ensemble. While some of these approaches can be generalized, they are not immediately comparable across prediction models from different classes, and do not bound how much any well performing model may rely on a variable.

The permutation-based VI measure from RFs forms the inspiration for our definition of MR (see Section 3.1). This RF VI measure has been the topic of empirical studies (Archer and Kimes, 2008; Calle and Urrea, 2010; Wang et al., 2016), and several variations of the measure have been proposed (Strobl et al., 2007, 2008; Altmann et al., 2010; Hapfelmeier et al., 2014). Procedures related to “Mean Difference Impurity,” another VI measure derived for RFs, have been studied theoretically by Louppe et al. (2013); Kazemitabar et al. (2017). All of this literature focuses on VI measures for RFs, or for individual trees. Our estimator for model reliance differs from the traditional RF VI measure (Breiman, 2001) in that we permute inputs to the overall model, rather than permuting the inputs to each individual ensemble member. Thus, our approach can be used generally, and is not limited to trees or ensemble models.

Outside of the context of RF VI, Zhu et al. (2015) propose an estimand similar to our definition of model reliance, and Gregorutti et al. (2015, 2017) propose an estimand analogous to $e_{\text{switch}}(f) - e_{\text{orig}}(f)$. These recent works focus on model reliance specifically when f is equal to the conditional expectation function of Y (i.e., $f(x) = \mathbb{E}[Y|X = x]$). In contrast,

we consider model reliance for arbitrary prediction models f . Datta et al. (2016) study the extent to which a model’s predictions are expected to change when a subset of variables is permuted, regardless of whether the permutation affects a loss function L . To our knowledge, connections between permutation-based importance and U-statistics have not been previously established.

In discussing the Rashomon effect and VI, Breiman et al. (2001) suggest that ensembling many well-performing models together may alleviate the Rashomon problem. However, this approach may only push the problem from the model level to the ensemble level, as there may be many different ensemble models that fit the data well.

The Rashomon effect has also been considered in several subject areas outside of VI, including those in non-statistical academic disciplines (Heider, 1988; Roth and Mehta, 2002). In the context of optimization under uncertainty, Tulabandhula and Rudin (2014) optimize a decision rule to perform well under the predicted range of outcomes from any well performing model. Statnikov et al. (2013) propose an algorithm to discover multiple Markov boundaries, i.e., minimal sets of covariates such that conditioning on any one set induces independence between the outcome and the remaining covariates. Nevo and Ritov (2015) report interpretations corresponding to a set of well-fitting, sparse linear models.

5 Illustrations with simulated data

To illustrate the concepts of MR, AR, and MCR, we consider a simulated sample where $X = (X_1, X_2) \in \mathbb{R}^2$, and $Y \in \{-1, 1\}$ is a binary group label. Our primary goal in this section is to build intuition for the differences between these three importance measures, and so we demonstrate them here only in a single sample. We focus on the empirical versions of our importance metrics (\widehat{MR} , \widehat{MCR}_- and \widehat{MCR}_+), and compare them against AR, which is typically interpreted as an in-sample measure (Breiman, 2001), or as an intermediate step to estimate an alternate importance measure in terms of variable rankings (Gevrey et al., 2003;

Olden et al., 2004).

We simulate $X|Y = -1$ from an independent, bivariate normal distribution with means $\mathbb{E}(X_1|Y = 1) = \mathbb{E}(X_2|Y = -1) = 0$ and variances $\mathbb{V}(X_1|Y = 1) = \mathbb{V}(X_2|Y = -1) = \frac{1}{9}$. We simulate $X|Y = 1$ by drawing from the same bivariate normal distribution, and then adding the value of a random vector $(C_1, C_2) := (\cos(U), \sin(U))$, where U is a random variable uniformly distributed on the interval $[-\pi, \pi]$. Thus, (C_1, C_2) is uniformly distributed across the unit circle.

Given a prediction model $f : \mathcal{X} \rightarrow \mathbb{R}$, we use the sign of $f(X_1, X_2)$ as our prediction of Y . For our loss function, we use the hinge loss $L(f, (x, y)) = (1 - yf(x))_+$, where $(a)_+ = a$ if $a \geq 0$ and $(a)_+ = 0$ otherwise. The hinge loss function is commonly used as a convex approximation to the zero-one loss $L(f, (x, y)) = 1[y \neq \text{sign}\{f(x)\}]$.

We simulate two samples of size 300 from the data generating process described above, to be used for training and testing respectively. Then, for the class of models used to predict Y , we consider the set of degree-3 polynomial classifiers

$$\begin{aligned} \mathcal{F}_{d3} = \{f_{\theta} : f_{\theta}(x_1, x_2) = & \theta_{[1]} + \theta_{[2]}x_1 + \theta_{[3]}x_2 \\ & + \theta_{[4]}x_1^2 + \theta_{[5]}x_2^2 + \theta_{[6]}x_1x_2 \\ & + \theta_{[7]}x_1^3 + \theta_{[8]}x_2^3 + \theta_{[9]}x_1^2x_2 + \theta_{[10]}x_1x_2^2; \quad \|\theta_{[-1]}\|_2^2 \leq r_{d3}\}, \end{aligned}$$

where we set r_{d3} to the value that minimizes the 10-fold cross-validated loss in the training data. Let \mathcal{A}_{d3} be the algorithm that minimizes the hinge loss over the (convex) feasible region $\{f_{\theta} : \|\theta_{[-1]}\|_2^2 \leq r_{d3}\}$. We apply \mathcal{A}_{d3} to the training data to determine a reference model f_{ref} . Also using the training data, we set ϵ equal to 0.10 multiplied by the cross-validated loss of \mathcal{A}_{d3} , such that $\mathcal{R}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d3})$ contains all models in \mathcal{F}_{d3} that exceed the loss of f_{ref} by no more than approximately 10%. We then calculate empirical AR, MR, and MCR using information from the test observations.

We begin by considering the AR of \mathcal{A}_{d3} on X_1 . Calculating AR requires us to fit two

separate models, first using all of the variables to fit a model on the training data, and then again using only X_2 . In this case, the first model is equivalent to f_{ref} . We denote the second model as \hat{f}_2 . To compute AR, we evaluate f_{ref} and \hat{f}_2 in the test observations. We illustrate this AR computation in Panel 1 of Figure 2, marking the classification boundaries for f_{ref} and \hat{f}_2 by the black dotted line and the blue dashed lines respectively, and marking the test observations by labelled points. Comparing the loss associated with these two models gives one form of AR – an estimate of the necessity of X_1 for the algorithm \mathcal{A}_{d3} . Alternatively, to estimate the *sufficiency* of X_1 , we can compare the reference model f_{ref} against the model resulting from retraining algorithm \mathcal{A}_{d3} only using X_1 . We refer to this third model as \hat{f}_1 , and mark its classification boundary by the solid blue lines in Figure 2.

Each of the classifiers in Panel 1 of Figure 2 can also be evaluated for its reliance on X_1 , as shown in Panel 3 of Figure 2. Here, we use \hat{e}_{divide} in our calculation of \widehat{MR} (see Eq 3.2). Unsurprisingly, the classifier fit without using X_1 (blue dashed line) has a model reliance of $\widehat{MR}(\hat{f}_2) = 1$. The reference model f_{ref} (dotted black line) has a model reliance of $\widehat{MR}(f_{\text{ref}}) = 3.25$. These values of \widehat{MR} each have an interpretation contained to a single model – they compare the model’s behavior under different data distributions, rather than the AR approach of comparing different models’ behavior on the same data distribution.

We illustrate MCR in Panel 2 of Figure 4. In contrast to AR, MCR is only ever a function of well-performing prediction models. Here, we consider the empirical Rashomon set $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d3})$ – the set of models with test loss no more than ϵ above that of f_{ref} . We show the classification boundary associated with 15 well-performing models contained in $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d3})$ by the gray solid lines. To evaluate MCR, we apply a combination of heuristic solvers from the `dfoptim` and `optimr` packages in R to minimize linear combinations of $\hat{e}_{\text{orig}}(f_{\theta})$ and $\hat{e}_{\text{divide}}(f_{\theta})$, as described in Section B of the supplement. This results in approximate MCR bounds (see Lemmas B.2 & B.7 in the supplement). We also show two of the models in $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d3})$ that respectively attain an empirical model reliance within 0.1% of these approximate bounds, i.e., models that approximately attain the highest and lowest possible reliance on X_1 . We denote

Example: AR, MCR & MR for polynomial classifiers

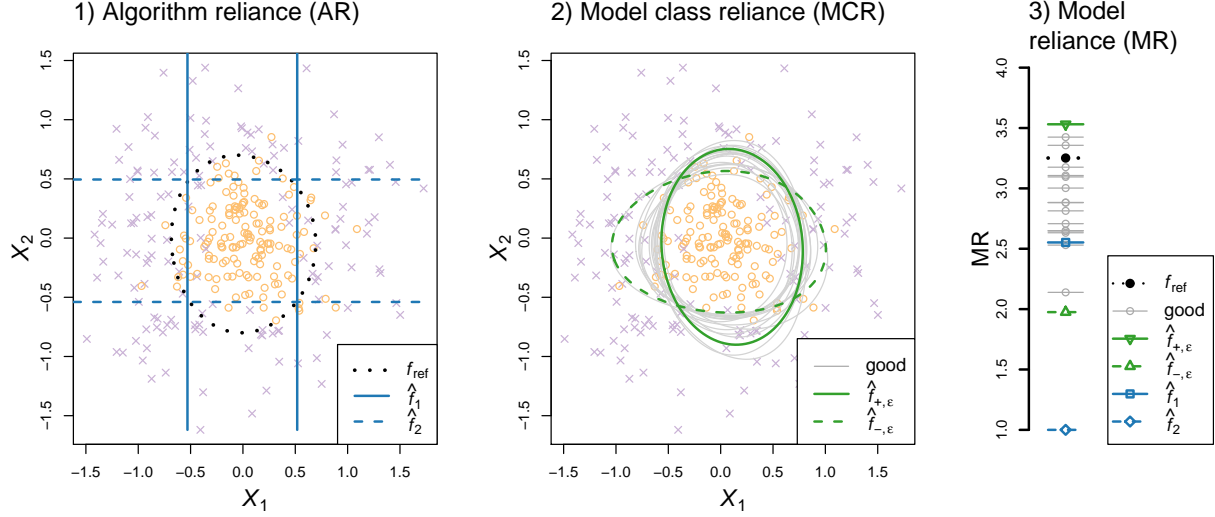


Figure 2: Example of AR, MCR & MR for polynomial classifiers – Panel 1 shows 300 draws from a simulated dataset, with the observed classification of each data point marked by “x” for $Y = 1$, and “o” for $Y = -1$. Classification boundaries for f_{ref} , \hat{f}_1 , and \hat{f}_2 are shown by the dotted, solid, and dashed lines respectively. For each classifier, points falling within the enclosed region receive a prediction of $Y = -1$, and points falling outside of the enclosed region receive a prediction of $Y = 1$. The models f_{ref} , \hat{f}_1 , and \hat{f}_2 are obtained on a separate simulated training dataset by respectively minimizing the hinge loss using both X_1 and X_2 as input, using only X_1 , and using only X_2 . Panel 2 shows the same simulated observations as Panel 1, along with classification boundaries for 15 well-performing models from the Rashomon set $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d3})$ marked by solid gray lines. Panel 2 also shows classification boundaries from $\hat{f}_{+, \epsilon}$ and $\hat{f}_{-, \epsilon}$, which approximately attain the highest and lowest reliance on X_1 respectively, among models in $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d3})$. Panel 3 shows the empirical model reliance on X_1 for each of the models in Panels 1 & 2.

these models as $\hat{f}_{+, \epsilon}$ and $\hat{f}_{-, \epsilon}$, and mark them by the solid green and dashed green lines respectively. For every model shown in Panel 2, we also mark its model reliance in Panel 3. We can then see from Panel 3 that \widehat{MR} for each model in $\hat{\mathcal{R}}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d3})$ is contained between $\widehat{MR}(\hat{f}_{-, \epsilon})$ and $\widehat{MR}(\hat{f}_{+, \epsilon})$, up to a small approximation error.

6 Data analysis: reliance of criminal recidivism prediction models on race and sex

Evidence suggests that bias exists among judges and prosecutors in the criminal justice system (Spohn, 2000; Blair et al., 2004; Paternoster and Brame, 2008; Danziger et al., 2011). In an aim to counter this bias, machine learning models trained to predict recidivism are increasingly being used to inform judges’ decisions on pretrial release, sentencing, and parole (Monahan and Skeem, 2016; Picard-Fritsche et al., 2017). Ideally, prediction models can avoid human bias and provide judges with empirically tested tools. But prediction models can also mirror the biases of the society that generates their training data, mistaking selectively collected data for reality. In the case of recidivism, if arrest rates across socioeconomic groups are not representative of underlying crime rate (Beckett et al., 2006; Ramchand et al., 2006; U.S. Department of Justice - Civil Rights Division, 2016), then bias can be created in both (1) the outcome variable, future crime, which is measured imperfectly via arrests or convictions, and (2) the covariates, which include the number of prior convictions on a defendant’s record (Corbett-Davies et al., 2016; Lum and Isaac, 2016). Over-reliance on model-based decision tools poses the danger of perpetuating bias and discrimination at scale. Further, when a prediction model’s behavior and mechanisms are an opaque black box, the model can evade scrutiny, and fail to offer recourse or explanations to individuals rated as “high risk.”

The issue we focus on in this section is that of transparency in prediction models. Given a hypothetical recidivism prediction model, we ask: how much does this model rely on race, sex, age, prior record, or charge severity, in order to predict well (MR, Section 3.1)? Comparing a given prediction model to similar models, we ask: how much, or how little, could any model from a prespecified class rely on these variables while still performing well (MCR, Section 3.3)? We also consider the more conventional approach of algorithm reliance, i.e., how much would the performance of a model-fitting algorithm suffer if the information in these variables was removed (AR, Section 3.2)? For each question, we consider reliance defined in terms of

Admissible variables	Inadmissible variables
number of priors, indicator of felony charge (versus misdemeanor), age, with linear spline points at: 20, 25, 30, and 40.	sex, race (indicator variables): Caucasian (intercept), African-American, Asian, Hispanic, Native American, Other.

Table 1: Covariates used from the Broward County criminal records dataset

in-sample prediction accuracy, using the empirical forms of MR, MCR and AR.

We analyze a public dataset of 6,172 defendants from Broward County, Florida. This dataset was compiled by ProPublica based on records from the Broward County Clerk’s Office, the Broward County Sheriff’s Office, and the Florida Department of Corrections. The outcome of interest (Y) is an indicator of 2-year recidivism as measured by arrests, which again is an imperfect measurement of criminal activity (Larson et al., 2016). Of the available covariates, we consider three variables which we refer to as “admissible.” These variables describe an individual’s age, their prior record, and the severity of the current charge. We also consider two variables which we refer to as “inadmissible,” an individual’s race (categorical) and sex (see Table 1). To answer the above questions, we compute the empirical MR, AR, and MCR on (1) all admissible variables, and on (2) all inadmissible variables.

As in Section 5, we define MR in terms of the hinge loss $L(f, (y, x)) = (1 - yf(x))_+$. For MCR, we consider the class of linear classifiers $\mathcal{F}_{d1} = \{f_{\theta} : f_{\theta}(x) = \theta_{[1]} + x'\theta_{[-1]}; \theta \in \mathbb{R}^{p+1}; \|\theta_{[-1]}\|_2^2 \leq r_{d1}\}$, where we determine r_{d1} by 50-fold cross-validation to optimally fit a subset \mathcal{S} of 1,000 observations. For AR, we define \mathcal{A}_{d1} as the model-fitting algorithm that minimizes empirical hinge loss among models in \mathcal{F}_{d1} , subject to the constraint that any input variable with variance equal to zero must have a coefficient of zero. Using the subset \mathcal{S} , we apply \mathcal{A}_{d1} to determine a reference model f_{ref} , and set ϵ equal to approximately 0.05 times the cross-validation loss of \mathcal{A}_{d1} on \mathcal{S} . Thus, $\mathcal{R}(\epsilon, f_{\text{ref}}, \mathcal{F}_{d1})$ is the subset of models in \mathcal{F}_{d1} with

expected loss exceeding that of the reference model f_{ref} by no more than approximately 5%. Using the held-out 5,172 observations, we then estimate the expected loss for f_{ref} , the model reliance for f_{ref} , the algorithm reliance for \mathcal{A}_{d1} , and the model class reliance for \mathcal{F}_{d1} . To calculate AR, we train \mathcal{A}_{d1} on the data subset \mathcal{S} , and evaluate its performance in the held-out observations. We compute MCR using the same approximations as in Section 5, based on the binary search procedure described in Section 3.3.3 (see Section B of the supplement).

In addition, we compute empirical MCR for the imputation residual of the inadmissible variables, after imputing their values based on admissible variables. As described in Section 3.4, this approximates the range of reliances on inadmissible variables among models that do not ignore admissible variables. We train imputation models on the data subset \mathcal{S} , using linear regression for continuous covariates, and multinomial logistic regression for categorical or binary variables. For categorical and binary variables, we define imputation residuals as the difference between the indicator of class membership and the imputed membership probability. We implement the same procedure to estimate MCR for the imputation residuals of the admissible variables, after imputing their values based on inadmissible variables.

Figure 3 shows the results of our analysis. We find that, overall, well-performing models rely more heavily on admissible variables than on inadmissible variables. For the reference model f_{ref} , the hold-out loss is $\hat{e}_{\text{orig}}(f_{\text{ref}}) = 0.74$. The empirical model reliance of f_{ref} on admissible variables is 1.44, exceeding the empirical reliance of f_{ref} on inadmissible variables, which is equal to 1.01. This means that the loss of f_{ref} will increase by a factor of 1.44 if the information in admissible variables is removed, but it will increase by only a factor of 1.01 if the information in inadmissible variables is removed. The algorithm \mathcal{A}_{d1} similarly has a higher empirical reliance on admissible variables than on inadmissible variables. From the empirical MCR measures, we find that any linear classifier in \mathcal{F}_{d1} cannot rely heavily on inadmissible information while still achieving an in-sample prediction loss no more than ϵ above the loss of the reference model, and may even have no reliance on inadmissible information (i.e., MR equal to 1). The 4th panel of Figure 3 shows MCR for the imputation

residual of the variable groups in Table 1, which, as expected, are lower than the MCR results in the 3rd panel. These results suggest that explicit model reliance on inadmissible information is unnecessary if not harmful for prediction accuracy, in addition to being unjust.

One important caveat is that models with no explicit reliance on race may instead rely on proxy variables that are correlated with race. In our dataset, prior misdemeanor convictions may act as such a proxy. A prior crime will only be observed in our dataset if it results in an arrest and a conviction. If comparable crimes committed by individuals in different demographic groups also differ in how likely they are to result in an arrest, this will lead to a systematic missing data problem (Corbett-Davies et al., 2016; Lum and Isaac, 2016). Evidence suggests that arrest rate disparities exist, particularly for misdemeanors and drug-related offenses (Beckett et al., 2006; Ramchand et al., 2006; U.S. Department of Justice - Civil Rights Division, 2016; Lum and Isaac, 2016), and so prior record may function partially as a proxy for race. A deeper analysis would benefit from subdividing the offense types in a defendant’s prior record. An additional caveat discussed by Kleinberg et al. (2016); Corbett-Davies et al. (2016) is that the fairness of a prediction model can be quantified according to multiple definitions, and that different definitions often form competing objectives.

7 Conclusion

In this paper, we propose a taxonomy of variable importance (VI) measures in order to help clarify differences between existing measures, and to introduce novel measures. For the permutation-based model reliance (MR) measure, we show that, conditional on the model, the conceptual framework of *iid* pairs and U-statistics can provide the sampling distribution of the MR VI estimator. We also derive a connection between MR and conditional causal effects, for the case of binary treatments, and between MR and the population covariance matrix, for the case of linear models. Building on MR, we propose model class reliance

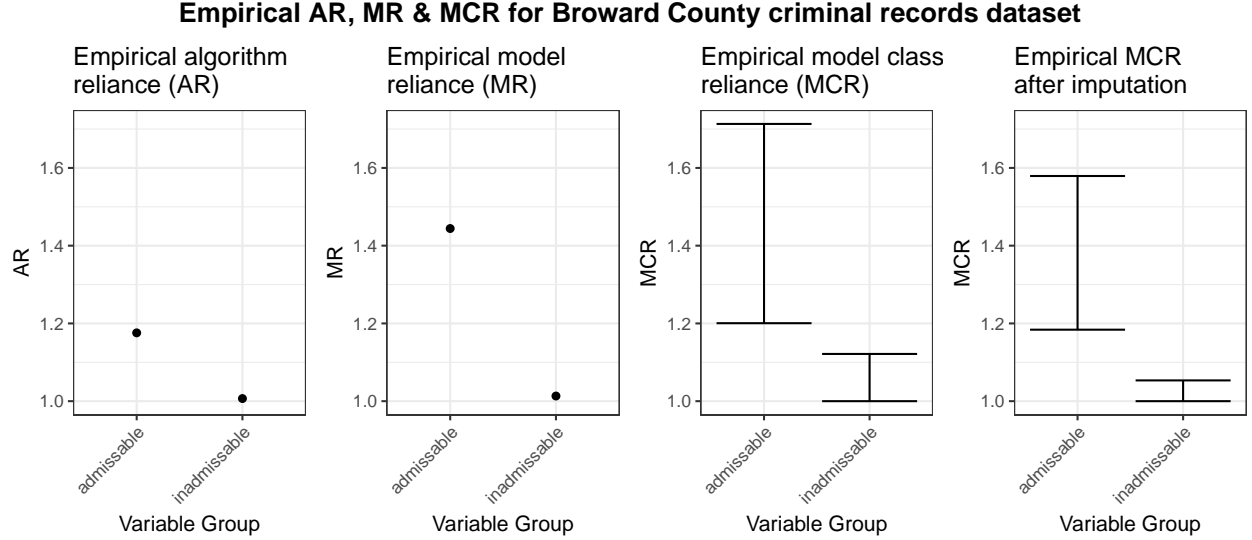


Figure 3: Empirical MR, AR, and MCR for Broward County criminal records dataset – Each measure is defined as a ratio, comparing the standard empirical loss against the loss when the variable of interest is removed (AR) or randomly reassigned (MR and MCR). For example, in the 2nd panel, the reliance of 1.44 on admissible variables indicates that the loss for the model f_{ref} increases by a factor of 1.44 if the information in the admissible variables is removed by a switch operation (see Section 3.1). In the 3rd panel, the range 1.00-1.12 indicates that for any model with empirical loss no more than ϵ above that of f_{ref} , the model’s loss increases by no more than 12% if race and sex are permuted. The 4th panel shows MCR for the imputation residual of the variable groups in Table 1.

(MCR) as the range of MR values for models in a “Rashomon set” – a set of models with high predictive accuracy. Our MCR approach of optimizing over Rashomon sets generalizes beyond the study of VI. Indeed, we show that similar approaches can be used to create finite-sample confidence intervals for almost any description of a best-in-class model. In future work, we aim to study the utility of empirical MCR for variable selection. Also of interest is to explore alternate methods for bounding population-level MCR based on either bootstrap or asymptotic inference.

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