Robust Output Analysis with Monte-Carlo Methodology

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In predictive modeling with simulation or machine learning, it is critical to assess the quality of estimated values through output analysis accurately. In recent decades output analysis has become enriched with methods that quantify the impact of input data uncertainty in the model outputs to increase robustness. However, most developments apply when the input data can be parametrically parameterized. We propose a unified output analysis framework for simulation and machine learning outputs through the lens of Monte Carlo sampling. This framework provides nonparametric quantification of the variance and bias induced in the outputs with higher-order accuracy. Our new bias-corrected estimation from the model outputs leverages the extension of fast iterative bootstrap sampling and higher-order influence functions. For the scalability of the proposed estimation methods, we devise budget-optimal rules and leverage control variates for variance reduction. Our numerical results demonstrate a clear advantage in building better and more robust confidence intervals for both simulation and machine learning frameworks.

Key words: Monte-Carlo simulation statistical analysis; bootstrap; robust non-parametric estimation

History:
1. Introduction

Estimating the output of a predictive logic has been studied for many decades in the statistics, simulation, and machine learning (ML) literature. Model error (output) estimation is used for two primary purposes (Raschka 2018): (a) evaluating the performance of the predictive logic on unseen data (model generalization) and (b) adjusting for the settings of the predictive model and comparing different predictive modeling classes with each other. In this paper, our focus is on achieving the first objective, (a), by correctly quantifying the effect of input data uncertainty (IU) on models’ outputs. Although goal (b) is not directly addressed, methods developed for goal (a) are shown to be effective in achieving the latter goals (see Section 1.2).

Let \( \theta(M|F) \) be the expected output of model \( M \) that is an instance in the family of models \( \mathcal{M} \) under input distribution \( F \). The above goals can be rephrased as (a) finding a robust estimate of \( \theta(M|F) \) that is less sensitive to uncertainties in the model and input data, i.e., with low bias and variance, and (b) finding the best model, \( M^* \), such that the error is minimized over a set of possible model input parameters, i.e., \( M^* = \arg\min_{M \in \mathcal{M}} \theta(M|F) \).

To motivate the benefit of our proposed robust output analysis, we provide two illustrative examples corresponding to (a) and (b).

1.1. Illustration I

We now illustrate the impact of the proposed method on system performance estimate (goal (a)). Take an \((s,S)\) inventory system for which demand data observations exist. We replicate the inventory system used in Koenig and Law (1985) with some modifications. The inventory policy in this system is to order up to \( S \) when the on-hand inventory falls below \( s \). The underlying distribution of demand per period for this example follows a Poisson distribution, which is unknown during simulation, but the simulation logic is known generating the total cost that consists of unit holding cost, ordering cost, and shortage cost over the simulation horizon. The simulation logic has a parameter, namely, the warm-up period, that can be tuned.
Three output analysis approaches are demonstrated over three input data sizes with \( R = 100 \). The points represent the average difference between the estimated cost and the observed cost.

For a given scenario, i.e., fixed \((s, S) = (20, 45)\), we have observed demand and the total cost for \( n \) periods and aim to test the accuracy of the simulation output confidence interval (CI) by including the observed expected total cost. This will help the stakeholder obtain a more reliable expectation of the magnitude of incurred costs. It will also be critical to comparing different scenarios, i.e., goal (b) (see Section 1.2 for a detailed example).

Conventionally, assuming that the distribution family of the demand is known, Poisson in this example, an input model is fitted to the observed demands. Then, the fitted distribution is incorporated into the simulation framework. In this case, \( Y(M|\hat{F}) \) are the simulation outputs, where in this example \( \hat{F} = F(\hat{\rho}) \) and \( \hat{\rho} \) is the MLE (maximum likelihood estimator) of the demand distribution input parameter. Then the desired expected total cost over the simulation horizon \( \theta(M|\hat{F}) = \mathbb{E}[Y(M|\hat{F})] \), will be estimated with \( \hat{\theta}(M|\hat{F}) = \bar{Y}(M|\hat{F}) := \frac{1}{R} \sum_{r=1}^{R} Y_r(M|\hat{F}) \), where \( R \) is the number of simulation runs. We refer to this output analysis as “crude”. However, the crude output analysis cannot quantify the input data variance when the data is limited or noisy.

The crude method can be enhanced by inflating its variance with the IU-induced variance \cite{Barton et al. 2018}. In this approach, \( Y(M|\hat{F}) \) is replaced with \( Y(M|\hat{F}^*) \), where in our example, \( \hat{F}^* = F(\hat{\rho}^*) \) represents the Poisson distribution with rate \( \hat{\rho}^* \), the MLE computed on the bootstrapped
resamples of the observed data. Using bootstrap of the data allows quantifying the model output total variance, including IU-induced variance. However, the IU-induced bias is neglected.

Despite the common assumption, IU is not unbiased (Song and Nelson 2019), meaning the output error due to uncertainty in specifying $F$ has a nonzero mean. Because there is no guarantee that the bias effect is the same across all input models and simulation runs, it is essential to quantify the IU-induced bias using bootstraps, $\hat{F}^*$. We propose a detailed method for debiasing the outputs and obtain $\hat{\theta}(M|F) = \frac{1}{R} \sum_{r=1}^{R} (Y_r(M|\hat{F}) - \hat{\text{bias}}_r(\hat{F}))$, where $\hat{\text{bias}}_r(\hat{F})$ is denoting the estimated bias on the $r$-th simulation run. Figure 1 demonstrates the effect of debiasing on the IU-inflated CI of the residual error on the total cost, i.e., the difference between the estimated average cost and the observed average cost, $\frac{1}{n} \sum_{i=1}^{n} y(D_i)$, where $D_i$ denotes the observed cost of the $i$-th period. Including zero in the CI means we have captured the desired value.

There is a clear advantage in debiasing, as it helps covering the desired value in the CI. We repeat this experiment with several input data sizes and observe that in the crude method, the performance does not necessarily improve with larger $n$ due to the discrepancy between the fitted distribution and the actual distribution. However, the improvement due to increased input data size is evident in the IU-inflated, and bias-corrected CI.

1.2. Illustration II

This illustration aims to demonstrate corrected CI’s impact on comparing different systems, which can be used for goal (b) in Section 1. Returning to the example introduced in the previous section, we compare our proposed debiased method with the state-of-the-art bias and variance estimation methods in the simulation literature. We demonstrate this by comparing the stationary trend between $(s,S)$ scenarios (Table 1), which is computed via 100 batch means of 30-period $(s,S)$ inventory simulation runs, against those trends from the output analysis with different techniques. The synthetically generated long-run trend with the batch means seeks to bury the dependence and nonstationarity in the outputs. Our goal is to recover the correct trend.
Table 1  The four scenarios of the \((s, S)\) inventory problem used for illustration II.

| Scenarios | 1  | 2  | 3  | 4  |
|-----------|----|----|----|----|
| \(s\)     | 20 | 20 | 20 | 20 |
| \(S\)     | 40 | 45 | 50 | 55 |

Figure 2  Comparing the 95% CI for two input data sizes and three competing methods. The role of bias is evident when comparing the different input data sizes. Although the bias decreases with larger input sizes, it plays an important role in correctly estimating the expected cost.

The experiment is run for two input sizes of 10 and 50, representing a 10-period simulation and 50-period simulation. Figure 2 reveals that the bias-corrected CI successfully captures the correct trend, and more resoundingly so with \(n = 50\). The input distribution greatly affects the crude method, as it does not allow any room for corruptions caused by IU. The distance between the crude CI and the observed cost roughly shows the magnitude is bias, which is in fact significant. The IU-inflated method performs better than the crude method; however, it is far from identifying the correct order between scenarios.

The bias-corrected method, even when \(n\) is limited, accurately estimates the bias and variance, successfully identifies the correct system, as well as the order between other systems. Such a powerful output analysis can then be used to calibrate the simulation model with a tuned warm-up period parameter. In the following sections of this paper, we will demonstrate how to achieve a bias estimator using fast iterated bootstrapping and higher order influence functions that readily apply to various problems.
1.3. Contributions

The practical stochastic model analysis platforms encompass ML and simulation. In ML, it is challenging to fit a model to the observed data during model construction and hyperparameter tuning. The goal is for the model to capture the underlying patterns but not mimic the input data so closely that it fails to generalize. For simulation, resembling challenges are calibrating the logic model and analysis of different scenarios for the system when there is limited observed data. Simulation literature refers to the latter as IU with a track of parametric methods for constructing inflated CIs on the estimated output. Computing CI requires an accurate estimation of model output bias and variance so that its actual coverage is close to its nominal value. This issue is direr in the ML problems due to high-dimensional input datasets and the additional impact of IU on the model. Fitting a parametric distribution to high-dimension data fails to capture the underlying uncertainty in the actual density generating function, $F$. We develop a non-parametric estimator for model output given the observed data empirical distribution, such that correct CI for any model are easily attainable. The proposed method can also be beneficial for big data problems; when due to computational expenses, the user can take smaller subsets of data and leverage the proposed bias-corrected CI to compensate for the loss of data.

We summarize the contributions of this paper as

- proposing a unified framework for data-driven output analysis by bridging stochastic simulation to ML predictive modeling;

- introducing non-parametric estimation methods for variance and bias of the model output utilizing the law of total variance, fast iterated bootstrapping, and non-parametric delta methods;

- computing the variance of the bias estimators and minimizing it using the control variate technique and optimal budget allocation derived from simulation methodology;

- defining a sampling-based algorithm for computing the ML model prediction error incorporating the mentioned bias and variance estimators in addition to out-of-bag sampling combined with $m$-out-of-$n$ bootstrapping;
demonstrating the benefits of employing the proposed approach on simulated datasets in both stochastic simulation and machine learning fields.

In the following sections, we first cover background literature on both ML and simulation techniques for output analysis in Section 2. Section 3 defines the proposed estimator and demonstrates its statistical properties. Then in Section 5 we elaborate on the nuances of ML model prediction estimation. Section 6 will compare the benefits of the proposed estimator with the existing benchmarks. Lastly, in Section 7 we conclude our discussion and point the interested audience to the future research directions.

2. Background

We now review the existing literature in simulation and ML output analysis. In simulation, $M$ is the model’s underlying logic, often independent of data except in model validation. On the other hand, in ML, $M$ represents the data-dependent model’s logic. In both $F$ is the input data distribution.

2.1. Stochastic Simulation

Output analysis has been widely studied under parametric and non-parametric distributions in simulation systems (Lam 2016, Barton 2012). Parametric output analysis limits the data to a known family of distribution, which may fail to encompass the actual characteristics of the input data. Given a parametric input distribution and utilizing Taylor expansion, Morgan et al. (2019) compute an estimator for bias due to unknown input distribution for the simulation output. However, their method does not generalize to non-parametric input models. Song and Nelson (2019) provide an extensive simulation output analysis under IU, where the bias and variance of the simulation models are studied considering parametric input models. They estimate the bias via regressing the model outputs versus the data distribution parameter. They show that the distribution between the input parameters and simulation output asymptotically follows a bi-variate normal, although with unclear validity for small data sizes ($n < 50$). Yang et al. (2021) suggests another novel parametric approach towards deconvoluting the bias of IU in estimating a conditional expectation by debiasing
the density of the input data. Density deconvolution refers to fitting a density to noisy observed data by separating the noise from the density function.

To the best of our knowledge, without any prior distributional assumption on the input data, there is no procedure to identify the bias due to input modeling. However, there are some noteworthy studies on estimating the variance of the simulation model output. Barton et al. (2018) present an optimized sampling method for variance estimation. They suggest a nested simulation framework with bootstrapping to capture the data variability. Furthermore, Lam and Qian (2019) propose an alternative variance estimator using non-parametric delta methods, i.e., influence functions. They estimate the variability of the output with respect to small changes in the empirical input distribution. Lam and Qian’s method can further be applied to estimating the gradient in optimization processes. We have previously developed a bias estimator for the output of the stochastic simulation models using sampling-based methods and influence functions (Vahdat and Shashaani 2021). Nevertheless, the estimated bias was not practical due to high variability. In this paper, we build on the previous bias estimator and reduce its variance by employing the variance reduction techniques. We also rigorously prove the validity of the proposed estimator.

Non-parametric estimation methods are better suited for high-dimensional settings and are more generalizable to various problems. However, they have some drawbacks. Non-parametric methods, usually based on data sampling, are computationally expensive, so they may not perform well for a limited computation budget (Fithian et al. 2014). In this paper, we propose an optimal allocation of the computation budget for the proposed bias and variance estimators to efficiently encompass the underlying uncertainty of the observed data into our estimation. Another drawback of non-parametric methods is their high dependence on the observed data (Lam 2021). We attempt to resolve this issue by implementing multi-level data sampling to reduce the dependency.

The benefits of model output analysis considering IU are not limited to evaluating the simulation models. An exciting application of IU that has been of focus recently is distributionally robust optimization (DRO). In DRO, minimizing the expected output of a model, typically considered in simulation optimization settings, \( \min_M \mathbb{E}_F[\theta(M|\hat{F})] \), is converted to a min-max alternate, where the optimal solution is found within the worst-case in an uncertainty set, \( \mathcal{F} \), i.e.,
min_{M} \{ \sup_{\hat{F} \in \mathcal{F}} \theta(M|\hat{F}) \}. To avoid confusion with $\hat{F}$ representing the empirical distribution, $\tilde{F}$ is used here to denote any random input model. The main challenge in DRO is finding an unbiased and reliable estimate for $\nabla_{\hat{F}} \theta(M|\tilde{F})$. Ghosh et al. (2018) employ Giles’ debiased estimator for the gradient in training ML models. The Giles’ method (Giles 2008, Blanchet and Glynn 2015) is a practical way of debiasing a function of expected values, $E_{\hat{F}}[\theta(M|\tilde{F})]$; however, it is only applicable when the function does not have an unbiased estimator, i.e., this method does not directly apply to sample average as an estimator of $E_{\hat{F}}[\theta(M|\tilde{F})]$. Lam and Zhang (2021) provide an unbiased estimator of stochastic gradient descent using only a few sample observations. Their proposed estimator utilizes score functions to cancel out the higher-order bias terms without explicitly characterizing the bias. In this paper, however, we introduce a bias estimator applicable to $E_{\hat{F}}[\theta(M|\tilde{F})]$ that can be directly used to guide the optimization.

2.2. Machine Learning

The ML literature often does not recognize learning model outputs as a function of the unknown input data distribution. The existing body of work generally propose methods solely for a limited set of learning models, i.e., linear regression. Shao (1996) and Rabbi et al. (2021) introduce bootstrap-based confidence intervals for variable coefficients in linear regression that take the unknown input data into account. Model agnostic output analysis relies primarily on “good” data sampling procedures that provide a robust estimate and address the conditional nature of the model output. Good data sampling is critical, especially when the magnitude of the desired performance is important.

Many sampling methods have been developed by statisticians; $k$–fold cross validation (Geisser 1975, Stone 1974), .632 bootstrapping, double bootstrap, out-of-bag bootstrapping, and leave-one-out bootstrap or LOOBoot (Efron and Tibshirani 1997, Efron 1983) are well-known methods widely used for predictive model error analysis. For a more extensive review of the bootstrap-based model output estimation techniques, we refer the interested readers to a survey by Austin and Tü (2004). While these methods’ estimates may be good enough for general model comparisons, they fail to deliver reliable output CI. As noted, reliable CI refers to confidence intervals that cover the true
values with high likelihood, i.e., high coverage probability. We propose a novel bootstrap-based sampling method for quantifying the model’s performance, resulting in an unbiased estimate with IU-inflated variance, thus more reliable CI with improved coverage probability. Some studies in statistical analysis provide sampling-based estimators of bias, but they are not utilized in stochastic simulation settings. Also, optimizing the variability of their bias estimators and its impact on reliability is taken for granted. Chang and Hall (2015) describes an exciting double bootstrapping approach, where the first level perturbs the input data and the second level varies previous level perturbed distributions. In this method, the second level only requires one replication.

Ultimately, augmenting ML performance estimation with Monte Carlo-based output analysis increases the reliability and robustness of ML’s associated optimization routines for model construction. Correctly estimating CI for the outputs gives us more accurate performance measures for a given input, which can tremendously help compare solutions and increase robustness.

3. Proposed Methodology

We define our unified problem statement for ML and simulation as estimating $\theta(M(F)|F)$ that measures the expected output of a logic model $M$ given the observed dataset, $D$, that follows the unknown distribution $F$. We use $M(F)$ to recognize that the logic can be determined (ML) or calibrated (simulation) with the input model. Denote the on-hand dataset with $D \in \mathbb{R}^{n \times (d+1)}$: $\{(z_i, y_i)\}_{i=1,…,n}$, each point of which represents one input data point, $z_i$, and its corresponding output, $y_i$. For ease of exposition, we simplify the model expected output with $\theta(F)$. The objective is to estimate $\theta(F)$, as closely as possible, despite that $F$ is unknown. Let an output of the model $M(F)$ be represented with $Y(F)$. Then we can write $\theta(F) = \mathbb{E}[Y(F)]$, or equivalently

$$Y(F) = \theta(F) + \epsilon(F),$$

where $\epsilon(F)$ is the stochastic error with mean 0.

Assuming that $\theta(\cdot)$ is a smooth function of $F$, and $F$ is fixed over time, we aim to find an efficient and robust estimator for $\theta(F)$ using replicated outputs $Y_r(F)$ for $r = 1, \cdots, R$. In practice $F$ can
be estimated with the empirical distribution of the data on hand,  
\[ \hat{F} = \frac{1}{n} \sum_{i=1}^{n} \delta_D(z_i), \]
where \( \delta_D(z) \) denotes the Dirac measure (takes value of 1, if \( z \in D \), and 0 otherwise) for point \( z \). In our analysis for ML type problem, the learning algorithm or model choice has no restriction, although we use linear regression in the numerical experiments. Our main reason for using linear regression is to make the computation less costly. We also will show that although linear regression may not be a good choice for the underlying system logic, with reliable output analysis, it can still successfully predict good/bad alternatives.

The point estimator for \( \theta(\hat{F}) \) is expressed as a sample average approximation (SAA) (Kleywegt et al. 2002) of \( R \) simulation outputs, denoted by \( Y_r(\hat{F}) \) for \( r = 1, \ldots, R \). We will set the optimal number of simulation runs in Section 4.3. Here simulation refers to an iterative process of generating independent replications of \( Y(\hat{F}) \). Hence,

\[
Y(\hat{F}) = \theta(F) + W(\hat{F}) + \epsilon(\hat{F}),
\]

where \( W(\hat{F}) \) is the random bias in the random output with \( \mathbb{E}[W(\hat{F})] = \beta(\hat{F}) = \theta(\hat{F}) - \theta(F) \).

**Remark.** Our original framework was to estimate \( \beta(\hat{F}) \) directly, but we soon found that estimator is in fact highly variable, in particular in the ML examples, and changed the debiasing framework to take effect for each single output observation.

This bias can be negligible if the number of observed data points is large (Hall 1986). However, in many complex systems, either data is not readily available or using all of the data can be computationally expensive and we can opt for smaller subsets of data. Both cases induce bias into estimation. Assuming simulation outputs are conditionally unbiased, the crude point estimator is

\[
\bar{Y}(\hat{F}) = \frac{1}{R} \sum_{r=1}^{R} Y_r(\hat{F}).
\]

Since only \( \hat{F} \) is attainable for estimation, therefore the bias \( \beta(\hat{F}) \) cannot be directly observed. We follow the bootstrap theory (Efron 1979), namely,

\[
\mathbb{E}_* [\theta(\hat{F}^*)] - \theta(\hat{F}) \approx \theta(\hat{F}) - \theta(F),
\]
with $E_*[\cdot]$ being the expectation with respect to the bootstraps distribution, $\hat{F}^*$ to provide an approximation for $\beta(\hat{F})$. In other words, bootstrap theory enables estimating the bias, without accessing $F$, with unlimited computation power. The random bias in (1) can be rewritten as

$$W(\hat{F}) = E_* \left[ Y(\hat{F}^*) - Y(\hat{F}) \mid \hat{F} \right] \Delta^*(\hat{F}) = \frac{1}{n^n} \sum_{b=1}^{n^n} \Delta_b^*(\hat{F}),$$

(3)

where $n^n$ is the number of overall unique bootstrap possibilities with a dataset of size $n$, and $\Delta_b^*(\hat{F}) := Y(\hat{F}_b^*) - Y(\hat{F}) \mid \hat{F}$ is the discrepancy between the random outputs with empirical and the $b$-th bootstrapped input distribution. In practice, it is not possible to enumerate $n^n$ combinations; we calculate the average over $B \ll n^n$ bootstrap samples and approximate the bias with

$$W(\hat{F}) \approx \bar{\Delta}^*(\hat{F}) := \frac{1}{B} \sum_{b=1}^{B} \Delta_b^*(\hat{F}) = \frac{1}{B} \sum_{b=1}^{B} \left( Y(\hat{F}_b^*) - Y(\hat{F}) \right).$$

(4)

The approximated bias in (4) represents the discrepancy between the model output given the empirical distribution and the actual distribution with accuracy of $O(n^{-1})$ (Hall 1986). We can enhance the approximated bias’s accuracy by characterizing the remaining error via an additional layer of bootstrap sampling. To rephrase it,

$$W(\hat{F}) = \bar{\Delta}^*(\hat{F}) + \gamma(\hat{F}),$$

(5)

where $\gamma(\hat{F})$ represents the discrepancy between the output with the bootstrapped distribution and the empirical distribution. We estimate $\gamma(\hat{F})$ in Section 4.2.1 by extending the work of Ouysse (2013). Ouysse (2013) utilizes fast iterative bootstrapping to estimate the bias to the order of $O(n^{-2})$. The word “fast” in its name is due to relying on only one bootstrap sample for estimating $\gamma(\hat{F})$, which results in computational efficiency.

In addition to bias, estimating the total variance and each of its contributing components is critical in building a correct CI and system diagnosis. When an estimate of each source of variability is known (stochastic noise or input data), one can effectively address the problematic component. For example, finding the input modeling process to contribute to the majority of variability can
change the decision of conducting more simulation replication to collecting more data. In this section, we estimate and decompose the total variance using the law of total variance. The variance of the defined point estimator in (2) is

$$\text{Var}(\bar{Y}(\hat{F})) = E_\hat{F} \left[ \text{Var}_Y \left( \bar{Y}(\hat{F}) | \hat{F} \right) \right] + \text{Var}_\hat{F} \left( E_Y \left[ \bar{Y}(\hat{F}) | \hat{F} \right] \right) = \frac{\sigma_Y^2}{R} + \sigma^2_{\hat{F}},$$

where the first term quantifies the simulation variance and the second term the variance associated with the input data.

The latter term in (6) can be estimated via three main approaches

I. parametric delta method, which limits the data to parametric distributions ($F$ follows a known distribution family) (Cheng and Holland 1997),

II. bootstrap sampling, where repeated samples of $\hat{F}$ is taken to estimate the variability among them (Barton 2012),

III. influence functions or non-parametric delta method (Lam and Qian 2019).
We explore the nonparametric methods (the last two items) toward estimating the variance. Both items I, and II, require instances of $\hat{F}$, resulting in an added bootstrap sampling from the observed data, which generates instances of empirical distribution that enables estimating the IU variance.

The analysis in the [2] and [4] was conditional on $\hat{F}$, however to include the variance estimation, we repeat them for each replication of $\hat{F}^\ast$. The added sampling layer results in a bias in the output functional estimator. We further expand the output definition to

$$Y(\hat{F}^\ast) = \theta(\hat{F}^\ast) + \epsilon(\hat{F}^\ast)$$

$$= \theta(F) + \theta(\hat{F}) - \theta(F) + W(\hat{F}^\ast) + \epsilon(\hat{F}^\ast)$$

$$= \theta(F) + \beta(\hat{F}) + \Delta^\ast(\hat{F}^\ast) + \gamma(\hat{F}^\ast) + \epsilon(\hat{F}^\ast),$$

(7)

where $\epsilon(\hat{F}^\ast)$ is the corresponding stochastic error, $W(\hat{F}^\ast)$ is the random bias of the output generated using the $\hat{F}^\ast$ input distribution (hence, $\mathbb{E}[W(\hat{F}^\ast)] := \theta(\hat{F}^\ast) - \theta(\hat{F})$), and $\beta(\hat{F})$ is the expected bias of using the empirical distribution instead of the true and unknown distribution – we will use a direct Taylor-like method later to estimate this.

Remark. Our original framework was to estimate $\beta(\hat{F}^\ast)$ similar to $\beta(\hat{F})$ and directly with the distributional Taylor expansion and gradient estimates of $\nabla_\theta \theta(\hat{F}^\ast)$ (with respect to $\hat{F}^\ast$, but we soon found that estimator in a deeper layer is in fact highly variable, in particular in the ML examples. Hence we changed the debiasing framework to take effect for each single output observation $Y(\hat{F}^\ast)$. This allows for common random numbers used to lower the debiased output’s variance significantly.

To clarify (7) further, as computing $W(\hat{F})$ requires $\hat{F}^\ast$ bootstraps in [4], so does computing $W(\hat{F}^\ast)$ a set of bootstrapped data from $\hat{F}^\ast$, which we will denote by $\hat{F}^{**}$ and computing $\gamma(\hat{F}^\ast)$ an additional bootstrap from the corresponding $\hat{F}^{**}$, which we will denote by $\hat{F}^{***}$. As clearly shown, each output observation can then be debiased by subtracting $\beta(\hat{F}) + \Delta^{**}(\hat{F}^\ast) + \gamma(\hat{F}^\ast)$ from it, which is the total bias induced by IU encompassing estimation and computing errors.

In the following subsections we detail the estimation methods for each term in (7). We explore estimating the bias using two non-parametric methods,
Figure 4 The proposed iterated bootstrap estimator is demonstrated.

1. fast iterated bootstrapping (FIB), and
2. higher order influence functions (HOIF).

FIB [Ouysse 2013], as briefly mentioned before, utilizes nested iterative bootstrapping to estimate the bias to the order of $O(n^{-2})$ with controlled computation cost. We explore augmenting FIB with simulation output analysis bridging the fields of simulation and ML. HOIF takes another approach toward estimating the bias; it estimates the second-order sensitivity of the output towards changes in the input distribution. On account of HOIF’s closed form estimator, it does not need additional bootstrap sampling. Nevertheless, HOIF requires known distributional behavior of the sampled data, so it can only be applied to estimating the $\beta(\hat{F})$, whereas FIB is easily applicable to $W(\hat{F}^*)$.

4. Estimation Procedures

This section elaborate on the methods used for estimating variance and bias that were briefly introduced in Section 3. Also, an optimized allocation of simulation budget is suggested.

4.1. Variance Decomposition

In this subsection, we quantify each component of the model output variability for better interpretability and decision making. To estimate $\sigma^2_{\hat{F}}$, we generate $B_1$ bootstrap samples from $\hat{F}$, denoted by $\hat{F}_{b_1}^*$ for $b_1 = 1, \cdots, B_1$. Each $\hat{F}_{b_1}^*$ is drawn with replacement from $\hat{F}$, is conditionally independent
of other resamples, and is treated as one sample of the empirical distribution, for which the simulation process is repeated $R$ times. The output of simulation replicate $r$ using bootstrap $b_1$ is denoted with $Y_r(\hat{F}_{b_1}^*)$. Then following the bootstrap theory (Efron 1979) we write $\sigma^2_{\hat{F}} \approx \text{Var}_s(\theta(\hat{F}^*))$, where $\text{Var}_s(\cdot)$ corresponds to the variance taken with respect to $B_1$ bootstraps.

With analysis of variance and (6) and assuming model outputs are conditionally unbiased, we can estimate the input distribution variance (Barton et al. 2018, Lam 2016). Note that $\text{Var}_s(\hat{Y}(\hat{F}^*)) = \text{Var}_s(\theta(\hat{F}^*)) + \mathbb{E}_s[\text{Var}(Y_r(\hat{F}^*)|\hat{F}^*)]/R$, that is estimated with

$$\hat{\text{Var}}_s(\theta(\hat{F}^*)) = \frac{1}{B_1 - 1} \sum_{b_1=1}^{B_1} (\hat{Y}(\hat{F}_{b_1}^*) - \bar{Y})^2 - \frac{1}{R} \frac{1}{B_1 (R - 1)} \sum_{b_1=1}^{B_1} \sum_{r=1}^{R} (Y_r(\hat{F}_{b_1}^*) - \bar{Y}(\hat{F}_{b_1}^*))^2,$$

where $\bar{Y}(\hat{F}_{b_1}^*) = \sum_{r=1}^{R} Y_r(\hat{F}_{b_1}^*)/R$ and $\bar{Y} = \sum_{b_1=1}^{B_1} \bar{Y}(\hat{F}_{b_1}^*)/B_1$. In (8) each variance is estimated with sum of squared residuals with respect to the variability source.

On the other hand, based on (7), $Y_r(\hat{F}^*)$ in (8) is biased. The unbiased estimate is represented with $\tilde{Y}_r(\hat{F}^*) = Y_r(\hat{F}^*) - \hat{\beta}(\hat{F}) - W_r(\hat{F}^*)$, where $\hat{\beta}(\hat{F})$ is an unbiased estimate of $\beta(\hat{F})$. We will discuss this estimator in Section 4.2.2 and in (21). We will then have

$$\text{Var}(\tilde{Y}_r(\hat{F}^*)) = \text{Var}(Y_r(\hat{F}^*) - \hat{\beta}(\hat{F}) - W_r(\hat{F}^*)|\hat{F}^*)$$
$$= \text{Var}(Y_r(\hat{F}^*)|\hat{F}^*) + \text{Var}(\hat{\beta}(\hat{F}) + W_r(\hat{F}^*)|\hat{F}^*) - 2\text{Cov}(Y_r(\hat{F}^*), \hat{\beta}(\hat{F}) + W_r(\hat{F}^*)), \text{IU-induced bias variability}$$

where $\text{Var}(Y_r(\hat{F}^*)|\hat{F}^*)$ is estimated in (8). Thus, we can estimate the total variability due to bias terms, including covariance between the bias and model output, knowing

$$\hat{\text{Var}}(\hat{\beta}(\hat{F}) + W_r(\hat{F}^*)) = \frac{1}{R - 1} \sum_{r=1}^{R} (Y_r(\hat{F}) - \bar{Y}(\hat{F}))^2$$
$$- \frac{1}{B_1 (R - 1)} \sum_{b_1=1}^{B_1} \sum_{r=1}^{R} (Y_r(\hat{F}_{b_1}^*) - \bar{Y}(\hat{F}_{b_1}^*))^2.$$

(9)

Each estimated variance above can identifies the contribution of its source (simulation, input data, or bias of input data) in the total variance and subsequently enhance the decision making.
4.2. Bias Estimation

Besides computing the variance of the output, we also need to quantify the bias, as described in (7). Bias can occur for two main reasons: the use of empirical distributions to quantify the error and the discrepancy between the true statistical and the estimated models. We only focus on the first bias term and leave the second one for future research.

In the previous section, in order to disintegrate the variance due to IU, we generated bootstrapped replications of the empirical distribution. We assume the expected model output is a smooth functional of input distribution and data observations are independent and identically distributed. Following the delta method a functional of the bootstrapped distributions converge to the functional of the actual distribution asymptotically, despite a non-negligible bias with limited simulation budget and data points (Van der Vaart 1998). In the subsequent sections, we explore the two methods of FIB and HOIF for estimating the bias terms defined in (7).

4.2.1. Fast Iterated Bootstrapping  We start by quantifying the bias due to bootstrapping, \( \beta(\hat{F}^*) \). Each simulation output given the sampled input is denoted by \( Y_r(\hat{F}^*_{b_1}) \) that is assumed to be a consistent estimator. We write the bootstrap estimate of bias as,

\[
\bar{\Delta}^{**}_r(\hat{F}^*_{b_1}) = \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r(\hat{F}^{**}_{b_1,b_2}) - Y_r(\hat{F}^*_{b_1}),
\]  

(10)

where \( B_2 \) is the number of bootstrap resamples taken at each \( B_1 \) input models for identifying \( W(\hat{F}^*_{b_1}) \). Also, \( \hat{F}^{**}_{b_1,b_2} \) represents the sample distribution taken with replacement from \( \hat{F}^*_{b_1} \). Note that in (10) the expectation is taken over another level of bootstrapping and hence the bias estimator itself is biased with the order of \( \mathcal{O}(n^{-2}) \) (Hall 1986).

Ouysse (2013) shows that we can estimate the bias of (10) with “fast” bootstrap sampling. Fast bootstrapping means that only one sample is taken for the second level to reduce the computation cost. Let \( \gamma_r(\hat{F}^{**}_{b_1,..}) \) be the bias of \( \bar{\Delta}^{**}_r(\hat{F}^*_{b_1}) \) due to limited \( B_2 \), and \( W_r(\hat{F}^*_{b_1}) = \bar{\Delta}^{**}_r(\hat{F}^*_{b_1}) + \gamma_r(\hat{F}^{**}_{b_1,..}) \) be the total bias, then similar to (5)

\[
W_r(\hat{F}^*_{b_1}) = \mathbb{E}_{**}[Y(\hat{F}^{**}_{b_1,..}) - Y_r(\hat{F}^*_{b_1})] = \bar{\Delta}^{***}_r(\hat{F}^{**}_{b_1,..}) + \gamma_r(\hat{F}^{**}_{b_1,..}),
\]

(11)
where $\Delta_r^{**}(\hat{F}_{b_1}) = \hat{E}_{***}[Y_r(\hat{F}_{b_1}) - Y_r(\hat{F}_{b_1})]$. Subtracting this equation from (11) achieves,

$$
\gamma_r(\hat{F}_{b_1}) = \hat{E}_{**}[Y_r(\hat{F}_{***}) - Y_r(\hat{F}_{***})] - \hat{E}_{**}[Y_r(\hat{F}_{***}) - Y_r(\hat{F}_{***})] \\
= \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r(\hat{F}_{b_1,b_2}) - Y_r(\hat{F}_{b_1,b_2}) - \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r(\hat{F}_{b_1,b_2}) + Y_r(\hat{F}_{b_1}) \\
= \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r(\hat{F}_{b_1,b_2}) - \frac{2}{B_2} \sum_{b_2=1}^{B_2} Y_r(\hat{F}_{b_1,b_2}) + Y_r(\hat{F}_{b_1}).
$$

We define the fast iterated bootstrap corrected estimator as,

$$
\hat{Y}_r(\hat{F}_{b_1}) + \hat{\beta}(\hat{F}) = Y_r(\hat{F}_{b_1}) - \Delta_r^{**}(\hat{F}_{b_1}) - \gamma_r(\hat{F}_{b_1}) \\
= Y_r(\hat{F}_{b_1}) + \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r(\hat{F}_{b_1,b_2}) - \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r(\hat{F}_{b_1,b_2}).
$$

We further conduct a t-test to validate the significance of bias before applying it to the model output. T-test is applicable to our bias, because it is only an average of random model outputs, following the central limit theorem. Define the t-statistic as,

$$
T = \frac{W_r(\hat{F}_{b_1})}{\frac{1}{B_2} \sum_{b_2=1}^{B_2} \left( \Delta_r^{**}(\hat{F}_{b_1,b_2}) + \gamma_r(\hat{F}_{b_1,b_2}) - W_r(\hat{F}_{b_1}) \right)^2}.
$$

If $|T|$ is greater than the critical values of Student-t distribution, we will overlook the bias.

### 4.2.2. Higher Order Influence Functions

In this subsection, we quantify $\beta(\hat{F}) = \theta(\hat{F}) - \theta(F)$ using Von-Mises expansion and influence functions [Van der Vaart 1998]. Von-Mises expansion is similar to the Taylor expansion with some modifications; define the function $\phi: t \to \theta(F + t(\hat{F} - F)\sqrt{n})$. We estimate $\phi(t)$ at $t = 0$ using the Taylor expansion as,

$$
\theta(F + t(\hat{F} - F)\sqrt{n}) = \theta(F) + t\nabla_F\theta(\hat{F} - F)\sqrt{n} + \frac{nt^2}{2}\nabla^2_F\theta(\hat{F} - F)^2 + O((t\|\hat{F} - F\|\sqrt{n})^3),
$$

where $\nabla_F\theta$ and $\nabla^2_F\theta$ are the first and second order directional derivatives of $\theta$. In Von-Mises expansion, $t$ is replaced with $1/\sqrt{n}$ which results in,

$$
\theta(\hat{F}) = \theta(F) + \nabla_F\theta(\hat{F} - F) + \frac{1}{2}\nabla^2_F\theta(\hat{F} - F)^2 + O(||\hat{F} - F||^3).
$$

(14)
Assuming a linear and continuous first-order derivative, we have 
\[ E[\nabla F \theta(\hat{F} - F)] = \nabla F \theta(\mathbb{E}[\hat{F} - F]) = 0. \]
Hence, taking an expectation with respect to \( F \) from (14) yields 
\[ E[\theta(\hat{F}) - \theta(F)] \approx E[\nabla^2 F \theta(\hat{F} - F)^2] / 2. \]

Provided that the desired functional is smooth, \cite{Efron2014} shows that based on the bootstrap theory \( \|\hat{F}^* - \hat{F}\| \to \|\hat{F} - F\| \) as the number of data points grow large, and similarly, \( \theta(\hat{F}^*) - \theta(\hat{F}) \to \theta(\hat{F}) - \theta(F) \). The smoothness assumption is valid in our case because \( \theta \) is the expectation of model error. Employing the smoothness of \( \theta \), we can estimate its first and second-order derivatives using the bootstraps already created for variance estimation. Consequently, we rewrite (14) using the empirical distribution and its random perturbation, \( \hat{F}^* \).

Each \( \hat{F}^*_b \) for \( b_1 = 1, \ldots, B_1 \), as explained in Section 4.1, is sampled from the empirical distribution of the on-hand dataset, \( \hat{F} \), with replacement and size \( m \leq n \). As noted by \cite{LamQian2021}, sampling less than the on-hand data size will help manage the computation cost while controlling the variance. We point out additional advantages of sub-sampling in ML application in Section 5.

Define the probability of selecting point \( i \) in \( \hat{F}^*_b \) as 
\[ N_{b_1,i} = \# \{ D_{b_1} = D_i \} \sim \text{binomial}(m, p_0) \] 
(15)
is the number of repeated samples of \( D_i \) in \( D_{b_1} \). In (15), \( p_0 = (1/n, \ldots, 1/n) \), and \( N_{b_1} \sim \text{Mult}(m, p_0) \).

Additionally, \( D_{b_1} \) represents the \( b_1 \)-th sample taken from \( D \). Note that \( \hat{F} \) and \( \hat{F}^* \) can be written as 
\[ \frac{1}{n} \sum_{i=1}^{n} \delta(z_i) \] and 
\[ \frac{1}{m} \sum_{i=1}^{n} N_{b_1,i} \], respectively. Then the Von-Mises expansion for an arbitrary \( b_1 \) is,
\[
\theta \left( \hat{F}^*_b \right) = \theta(\hat{F}) + \sum_{i=1}^{n} \nabla F \theta \left( \frac{N_{b_1,i}}{m} - \frac{\delta(z_i)}{n} \right) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \nabla^2 F \theta \left( \frac{N_{b_1,i}}{m} - \frac{\delta(z_i)}{n} \right) \left( \frac{N_{b_1,j}}{m} - \frac{\delta(z_j)}{n} \right) 
\]
\[
= \theta(\hat{F}) + \sum_{i=1}^{n} \nabla F \theta \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \nabla^2 F \theta \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,j}}{m} - \frac{1}{n} \right), 
\]
where the second equation simplifies the first by limiting the summation to the available data points and replacing \( \delta \) with 1.
It remains to propose an unbiased estimator for $\nabla_p \theta$ and $\nabla^2_p \theta$. We employ score functions to develop the desired estimators. Lam and Qian (2019) propose an unbiased estimator for $\nabla_p \theta$ at point $z_i$ using score functions,

$$\widehat{IF}_1(z_i; \hat{F}) = \frac{1}{B_1} \sum_{b_1 = 1}^{B_1} \frac{1}{R} \sum_{r = 1}^{R} Y_r \left( \hat{F}_{b_1}^* \right) S_i^{(1)} \left( \hat{F}_{b_1}^* \right),$$

where

$$S_i^{(1)} \left( \hat{F}_{b_1}^* \right) = \frac{n - 1}{n \text{Var}(N_{b_1,i}/m)} \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) = mn \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right)$$

is the score function. They show that $E[\widehat{IF}_1(z_i; \hat{F}) | \hat{F}] = \nabla_p \theta$, hence it is unbiased. We build on their approach to provide an unbiased estimator for $\nabla^2_p \theta$, which then can be used for the bias estimation.

Note that $\nabla^2_p \theta$ is a bilinear mapping, so for a given pair of distinct points $z_i$ and $z_j$, we define the estimator as,

$$\widehat{IF}_2(z_i, z_j; \hat{F}) = \frac{1}{B_1} \sum_{b_1 = 1}^{B_1} \frac{1}{R} \sum_{r = 1}^{R} Y_r \left( \hat{F}_{b_1}^* \right) S_{i,j}^{(2)} \left( \hat{F}_{b_1}^* \right) + \lambda \hat{Y}_r(\hat{F}) + \lambda \eta \hat{IF}_1(z_i; \hat{F}),$$

where

$$S_{i,j}^{(2)} \left( \hat{F}_{b_1}^* \right) = \lambda \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,j}}{m} - \frac{1}{n} \right),$$

and

$$\frac{2}{\lambda} = \frac{m(m-1)(m-2)(m-3)}{m^4 n^2} + \frac{m(m-1)(m-2)}{m^3 n^3} \left( \frac{5n}{m} - 4n \right)$$

$$+ \frac{m(m-1)}{n^2 m^2} \left( \frac{4}{m^2} + \frac{8}{mn} - \frac{8}{mn^2} + 6 \right) - \frac{4}{mn^3} \frac{3}{n^2} - \frac{2}{m^3 n} + \frac{5}{mn^2},$$

$$= 10 \frac{mn^2}{m^2 n^2} - \frac{8}{mn^3} - \frac{8}{mn^4} - \frac{8}{m^2 n^3} + \frac{8}{m^2 n^4} - \frac{2}{m^3 n} = \frac{10}{mn^2} + O(n^{-4}).$$

Hence $\lambda \approx -1/5 \text{Cov}(N_{b_1,i}/m, N_{b_1,j}/m)$ and

$$\eta = \frac{m(m-1)(m-2)}{m^3 n^2} + \frac{m(m-1)}{m^3 n^3} \left( \frac{2}{m} - 3 \right) + \frac{2}{mn} + \frac{4 - n}{n^3}$$

$$= \frac{7}{m^2 n^2} - \frac{2}{mn} + \frac{2}{m^3 n^3} + \frac{4}{n^3} = - \frac{6}{mn^2} + \frac{4}{n^3} + O(n^{-4}),$$

that can be simplified to $\eta \approx 6 \text{Cov}(N_{b_1,i}/m, N_{b_1,j}/m) + 4E[N_{b_1,i}/m]^3$. We prove that the proposed estimator, $\widehat{IF}_2(z_i, z_j; \hat{F})$, is unbiased.
Theorem 1. \( \widehat{IF}_2(z_i, z_j; \hat{F}) \) defined in [17] is an unbiased estimator of \( \theta'' \).

Hence the bias estimate can be written as,
\[
\mathbb{E}_*[\theta(\hat{F}^*) - \theta(\hat{F})] = \mathbb{E}_* \left[ \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \widehat{IF}_2(i, j; \hat{F}) \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,j}}{m} - \frac{1}{n} \right) \right]
\]
\[
= \frac{1}{2} \mathbb{E}_* \left[ \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{r=1}^{R} \widehat{Y}_r(\hat{F}^*) S_{i,j}^{(2)} \left( \hat{F}^* \right) - \hat{F}_1 \left( z_i \right) \right]
\]
\[
= \frac{\lambda}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \text{Cov}_* \left( \frac{1}{R} \sum_{r=1}^{R} \widehat{Y}_r(\hat{F}^*), \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right)^2 \left( \frac{N_{b_1,j}}{m} - \frac{1}{n} \right)^2 \right) + O(m^{-2}n^{-4}).
\]

We can show that as \( n \) goes to infinity, the variance of \( \widehat{IF}_2 \) becomes unbounded (\( \text{Var}(\widehat{IF}_2) = O(n^5) \)). This means that in smaller datasets, we achieve a more stable estimator of bias than in larger datasets, which is not detrimental as the bias decreases with more data points. However, by utilizing the control variate technique, we can further reduce the variance. We use the \( \widehat{IF}_1 \) as the control variate statistic, since its expectation and variance are known. The control variate is our novelty in enhancing the HOIF bias estimator from its original variation in Efron (2014). It remains to compute the optimal coefficient of variance, that is equal to \( c^* = -\text{Cov}(\widehat{IF}_2(\hat{F}), \widehat{IF}_1(\hat{F}))/\text{Var}(\widehat{IF}_1(\hat{F})) \).

Theorem 2. The optimal coefficient of variance \( c^* = -\frac{\text{Cov}(\widehat{IF}_2(\hat{F}), \widehat{IF}_1(\hat{F}))}{\text{Var}(\widehat{IF}_1(\hat{F}))} \) can be approximate with
\[
-0.2 \left( n - \frac{1}{m} + \frac{2}{mn} + 1 \right) + O(m^{-2}n^{-2})
\]
due to
\[
\text{Cov}_*(\widehat{IF}_2(\hat{F}), \widehat{IF}_1(\hat{F})) \approx \frac{\widehat{Y}(\hat{F})^2}{5} \left( 2 + mn - n + mn^2 + \frac{6}{mn} - \frac{6}{mn^2} - \frac{4}{n^2} + \frac{4}{n^3} \right).
\]

Here we drop the \( z_i \) and \( z_j \) from the influence function estimators to generalize the results for any point.

Following these results, the final bias estimator becomes for a given \( b_1 \) is
\[
\hat{\beta}(\hat{F}) \approx (-1.2 \text{Cov}(N_{b_1,i}/m, N_{b_1,j}/m))
\]
Remark. Viewing each bootstrapped sample as one simulation replication, the expected bias in (20) is the same as second order linear regression coefficient of outputs with respect to the empirical cdf. For more intuition refer to Lin et al. (2015).

4.3. Optimal Allocation

Fixing the simulation effort $N = B_1 R B_2$, with the goal of having the simulation effort independent of the dataset size ($n$), one can find the optimum allocation of resources. Lam and Qian (2021) finds the best allocation for a nested simulation problem where sub-sampling has been incorporated into the outer simulation level. They prove that the optimum in the sense of minimizing the mean squared error of variance estimator is,

$$m^* = \Theta(N^{1/3}) \quad \text{if } 1 \ll N \leq n^{3/2},$$

$$\Theta(\sqrt{n}) \leq m^* \leq \Theta(\max(1, N/n)) \quad \text{if } N > n^{3/2},$$

which is translated, in our case, to

$$R^* B_2^* = \Theta(m^*), B_1^* = \frac{N}{R^* B_2^*}.$$  

We further complete the analysis by finding the optimum allocation by minimizing the variance of the bias estimator introduced in Section 4.2. The conditional variance of the simulation bias for arbitrary $b_2$ and $b_2'$ is

$$\text{Var}_r \left( \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r \left( \hat{F}_{b_1,b_2}^{**} \right) - Y_r \left( \hat{F}_{b_1,b_2}^{***} \right) \right) = \frac{1}{B_2} \text{Var}_r \left( Y_r \left( \hat{F}_{b_1,b_2}^{**} \right) - Y_r \left( \hat{F}_{b_1,b_2}^{***} \right) \right)$$

$$- \frac{B_2 - 1}{B_2} \text{Cov} \left( Y_r \left( \hat{F}_{b_1,b_2}^{**} \right), Y_r \left( \hat{F}_{b_1,b_2}^{***} \right) \right),$$

which can be rephrased as a function of $\text{Var} \left( Y \left( \hat{F}_{b_1}^* \right) \right)$ using the sample variance of bootstraps.

Theorem 3. Variance of the bias estimator in Section 4.2 is

$$\text{Var}_r \left( W_r(\hat{F}_{b_1}^*) \right) = \frac{\sigma^2(2m^* - 1)}{B_2(m^*)^2} \left( 1 + \frac{1}{B_2} \right) + \frac{(B_2 - 1)\sigma^2}{B_2 m^*} \left( 1 + \frac{B_2 - 1}{B_2} \right) - 2 \frac{\sigma^2}{m^*}.$$
Ensuring that the variance of bias is in the same order as the variance of the sample average of bootstrap replications of the simulation results in,

\[ B_2^* = \Theta \left( \left( \frac{3(m^*)^2}{m^* + 1} \right)^{1/3} \right), \]

subsequently \( R^* = \Theta \left( \frac{m^*}{B_2^*} \right). \)

5. Notes on Machine Learning Output Analysis

A critical class of data-driven problems where the proposed method is directly applicable is predictive ML models. In building a ML model, the model’s performance dramatically depends on the dataset used. For instance, if the training dataset is noisy and future data observations vary significantly from the input data, most ML models fail to achieve good prediction accuracy. Practitioners use different data-splitting measures to capture the conditional performance of ML models on the training data. In this section, we define a data sampling and splitting procedure derived from nested simulation settings in simulation (Sun et al. 2011) that results in bias-corrected CI.

We define the model output \( Y(\cdot) \) as the squared error between the ML model prediction and the observed response for all data points being predicted. The error must be computed on points not used for model training to avoid overfitting (Shashaani and Vahdat 2022). Here nested simulation refers to iterated data sampling defined in Sections 4.1 and 4.2 for estimating the output bias and variance. Using each sampled distribution, \( \hat{F}_{b_1}^* \), one model is fit, and its error on another set is calculated as the desired output. The nested simulation needs identically distributed (i.d.) and consistent model accuracy estimates. To obtain i.d. replicates, we define \( \hat{F}_{b_1}^* \) as the distribution of the sub-samples, \( m \)-out-of-\( n \) bootstrapping, with replacement for \( b_1 = 1, \ldots, B_1 \) (Shao 1996).

As shown in the ML and statistics literature (Breiman 2001, Rabbi et al. 2021), using out-of-bag samples improves the model accuracy estimation and decreases the bias. We combine the two methodologies, where the model’s performance is estimated on a \( m \)-out-of-\( n \) bootstrap sample evaluated on the out-of-bag points.

In the proposed algorithm, the model output, \( Y \), is calculated via a weighted average of squared residuals. We denote the ML model and the dataset it is trained on with \( M_D \), where \( D \) is the train
Table 2  Description of the data generating functions. The noise added to each function, \( \epsilon \), follows Normal distribution with mean zero and standard deviation 3 in the low noise and standard deviation 6 in the high noise cases. All independent variables, \( z_1, z_2, \) and \( z_3 \) follow gamma distribution with shape parameters 2, 5, and 3 and rate parameters 1, 2, and 1, respectively. The simulated datasets have 100 observations.

| Regression Type | Linear | Polynomial | Complex |
|-----------------|--------|------------|---------|
| Formula         | \( y = 5z_1 + z_2 + 2z_3 + \epsilon \) | \( y = z_1^2 + z_1 \times z_2 + z_2^2 + \epsilon \) | \( y = 5/\sqrt{z_1} + z_2 + 1/z_3 + \epsilon \) |

data. Also, to show the predicted value of the trained model on a data point, \( D_i \), we use \( M_D(D_i) \).

Having in mind Figure 3 and 4 that demonstrate the required multi-level sampling for estimating bias and variance, we summarize our ML sampling algorithm in Algorithm 1. Each output shown on Figure 4 requires a pair of non-overlapping train and test set. We use the input distribution of \( Y \) for testing, as the model error is calculated on them, and the holdout for training the model.

In Algorithm 1, we use the first random sample for testing the model, rather than building the model, which is essential in maintaining identically distributed error estimates for each data point [Vahdat and Shashaani 2022]. Taking the first sample as the testing set results in having conditionally independent model performance estimates. Further, we maintain the sub-sampling ratio \( \kappa = m^*/n \) throughout to ensure optimized computational efficiency (see Section 4.3).

6. Numerical Experiments

This section demonstrates the applicability of the proposed method in machine learning. The ML case study estimates the model prediction mean squared error on the test set. We use three simulated datasets, where the true model error is known. In this experiment various methods in estimating the model error are compared with each other. The role of the input data size and optimal budget allocation introduced in section 4.3 are studied.

We evaluate the performance of the proposed output analysis method by letting the under study functional be a machine learning regression model, where the purpose is to provide a correct confidence interval for the model mean squared error estimate. We conduct the experiment using three simulated data generating functions with two levels of noise added to the response to capture different functional structures and difficulty levels (see Table 2).

We compare our proposed confidence interval with and without optimal budget allocation with sampling-based methods commonly used in practice, leave one out bootstrap (LOOBoot), and
Algorithm 1 Sampling Algorithm For ML Error Estimation

Initialize: Given ML learning algorithm, dataset $D$ of $n$ unique data points, and simulation budget $N$, compute the optimal allocated budget for $B_1^*, R^*$, and $B_2^*$, and sub-sampling size $m^*$ using $N$, (22), and Theorem 3. Set $\kappa = m^*/n$.

for sample $b_1 = 1, 2, \cdots, B_1^*$ do

Draw $D_{b_1}$ from $D$ with replacement and size $m^*$.

Define $N_{b_1, i} = \#\{D_{b_1} = D_i\} \forall i = 1, 2, \cdots, n$.

for simulation $r = 1, 2, \cdots, R^*$ do

Draw a test sample $D_{b_1, r}$ from $D_{b_1}$.

Train model $M$ on $D_{b_1, (r)} = D_{b_1} \setminus D_{b_1, r}$.

Define $N_{b_1, r, i} = \#\{D_{b_1, r} = D_i\}$, and $I_{b_1, r, i} = I(D_{b_1, r, i} \in D_{b_1, r} \& D_{b_1, r, i} \notin D_{b_1, (r)}) \forall i$. Calculate the model output with

$$Y_{r}(\hat{F}_{b_1}^*) = \frac{1}{\sum_{i=1}^{n} I_{b_1, r, i} N_{b_1, r, i}} \sum_{i=1}^{n} I_{b_1, r, i} N_{b_1, r, i} \left( D_{b_1, r, i} - M_{D_{b_1, (r)}}(D_{b_1, r, i}) \right)^2.$$ \hspace{1cm} (23)

Bias Estimation:

for bootstrap $b_2 = 1, \cdots, B_2^*$ do

Draw $D_{b_1, r, b_2}$ from $D_{b_1, r}$ of the size $\kappa \times |D_{b_1, r}|$.

Train the model $M_{D_{b_1, r, (b_2)}}$ whose outputs on $D_{b_1, r, b_2}$ are $Y_{r}(\hat{F}_{b_1, b_2}^{**})$ following (23).

Draw $D_{b_1, r, b_2, 1}$ from $D_{b_1, r}$ of the size $\kappa^2 \times |D_{b_1, r}|$.

Train the model $M_{D_{b_1, r, (b_2), 1}}$ whose outputs on $D_{b_1, r, b_2, 1}$ are $Y_{r}(\hat{F}_{b_1, b_2}^{***})$ following (23).

end

Compute the debiased output, $\tilde{Y}_{r}(\hat{F}_{b_1}^*)$, with (12).

Check for significance of bias estimate via the t-statistic defined in (13).

end

Return: The IU-induced bias with (21), total variance with (8), and the bias-corrected CI.
Table 3  
With the total simulation budget of 1000, the probability of correct coverage is calculated over 100 replications. The first row is the proposed method and the second row is the proposed method with optimal budget allocation. The best coverage in each experiment is bolded.

| Regression Type                           | Linear | Polynomial | Complex |
|------------------------------------------|--------|------------|---------|
| Noise Variance                           | low    | high       | low     | high   |
| Budget-optimal bias-corrected CI coverage| 0.83   | 0.85       | 0.31    | 0.15   |
| Bias-corrected CI coverage               | 0.76   | 0.76       | 0.35    | 0.11   |
| IU-inflated Barton CI coverage            | 0.33   | 0.33       | 0.00    | 0.06   |
| IU-inflated Lam-Qian CI coverage          | 0.75   | 0.71       | 0.00    | 0.00   |
| LOOBoot CI coverage                       | 0.15   | 0.00       | 0.02    | 0.03   |
| Repeated CV CI coverage                   | 0.10   | 0.05       | 0.02    | 0.00   |

We keep the simulation budget fixed to 1000 for all cases to provide a fair ground for comparison. Table 3 compares the coverage probability for each method over the mentioned ML problems with two noise levels. The coverage probabilities are computed over 100 replications. We can observe that the bias-corrected CI significantly outperform the competitors. Lam and Qian, and Barton’s CI perform relatively better than repeated CV and LOOBoot in complex and linear functions. Moreover, we can improve the coverage probability with optimized budget allocation. Figure 5 demonstrates the CI for one replication.

7. Concluding Remarks

This paper showed the significance of incorporating bias and variance estimation in the model output analysis. We emphasize this matter via two common practical problems of machine learning...
Figure 5  Each panel shows the 95% CI for the competing methods for different data generating functions and rows are for high in each column. The dashed lines show the expected value.

and stochastic simulation. We bridge between the two fields providing a new playground for future research in the interconnection of ML and simulation.

We focused on non-parametric estimation methods to keep our results generalizable to data-driven problems. Furthermore, we addressed the computation inefficiency of non-parametric methods with an optimal budget allocation, which facilitates us to keep the computing budget the same while estimating the bias and variance of the model output. However, we do not include the model building cost in our computation budget, which can potentially be a drawback if a more complex model is fit. This problem can be addressed by restricting the non-parametric assumption to replace the bias estimator with a less number of resampling (Lin et al. 2015), which we leave for future research.

Viewing ML as a simulation clarifies the propagation of bias of data into output. Without prediction bias, the estimates of future outcomes of a decision can mislead the decision-maker into choosing a worse and riskier option. One of the future research paths of interest would be incorporating the proposed estimator into data-driven optimization problems.
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Appendix A: Theorem Proofs

A.1. Proof of Theorem 1

Proof.

\[ \mathbb{E}_Y \left[ \hat{I}_2^Y \left( z_i, z_j; \hat{F} \right) \mid \hat{F} \right] = \mathbb{E}_Y \left[ \frac{1}{B_1} \sum_{b_1=1}^{B_1} \frac{1}{R} \sum_{r=1}^{R} \hat{Y}_r \left( \hat{F}_{b_1}^* \right) S_{i,j}^{(2)} \left( \hat{F}_{b_1}^* \right) + \frac{\lambda \bar{Y}_r(\hat{F})}{m n^2} - \lambda \eta \bar{I}_1 \left( z_i; \hat{F} \right) \right] 
\]

\[ = \frac{1}{B_1} \sum_{b_1=1}^{B_1} \frac{1}{R} \sum_{r=1}^{R} \mathbb{E}_Y \left[ \hat{Y}_r \left( \hat{F}_{b_1}^* \right) S_{i,j}^{(2)} \left( \hat{F}_{b_1}^* \right) \right] - \mathbb{E}_Y \left[ \lambda \eta \bar{I}_1 \left( z_i; \hat{F} \right) \right] 
\]

\[ = \mathbb{E} \left[ \hat{Y}_r(\hat{F}) \lambda \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,j}}{m} - \frac{1}{n} \right) + \frac{\lambda \bar{Y}_r(\hat{F})}{m n^2} - \lambda \eta \nabla_\hat{F} \theta \right] 
\]

\[ = \lambda \bar{Y}_r(\hat{F}) \text{Cov} \left( \frac{N_i}{m}, \frac{N_j}{m} \right) + \nabla_\hat{F} \theta \lambda \mathbb{E} \left[ \sum_{i'=1}^{n} \left( \frac{N_{i'}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,j}}{m} - \frac{1}{n} \right) \right] 
\]

\[ + \frac{1}{2} \nabla^2_\hat{F} \lambda \mathbb{E} \left[ \sum_{i'=1}^{n} \sum_{j'=1}^{n} \left( \frac{N_{i'}}{m} - \frac{1}{n} \right) \left( \frac{N_{j'}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,i}}{m} - \frac{1}{n} \right) \left( \frac{N_{b_1,j}}{m} - \frac{1}{n} \right) \right] 
\]

\[ + \frac{\lambda \bar{Y}_r(\hat{F})}{m n^2} - \lambda \eta \nabla_\hat{F} \theta \]
A.2. Proof of Theorem 2

Proof.

\[
\text{Cov}_* \left( \hat{I}_1^2(\hat{F}), \hat{I}_1(\hat{F}) \right) = \text{Cov}_* \left( \hat{Y}(\hat{F})S_{i,j} + \frac{\lambda}{mn^2} - \lambda \eta \hat{Y}(\hat{F})S_{i}, \hat{Y}(\hat{F})S_{i} \right)
\]

\[
= \text{Cov}_* \left( \hat{Y}(\hat{F})S_{i,j}, \hat{Y}(\hat{F})S_{i} \right) + \frac{\lambda}{mn^2} \text{Cov}_* \left( Y(\hat{F}), \hat{Y}(\hat{F})S_{i} \right)
\]

\[
- \lambda \eta \text{Cov}_* \left( \hat{Y}(\hat{F})S_{i}, \hat{Y}(\hat{F})S_{i} \right)
\]

\[
= \hat{Y}(\hat{F})^2 (mn\lambda) \text{Cov} \left( \left( \frac{N_i}{m} - \frac{1}{n} \right) \left( \frac{N_j}{m} - \frac{1}{n} \right), \left( \frac{N_i}{m} - \frac{1}{n} \right) \right) - \lambda \eta \text{Var} \left( \hat{Y}(\hat{F})S_{i} \right)
\]

\[
= \hat{Y}(\hat{F})^2 (mn\lambda) \left( E \left[ \left( \frac{N_i}{m} - \frac{1}{n} \right)^2 \left( \frac{N_j}{m} - \frac{1}{n} \right) \right] - E \left[ \left( \frac{N_i}{m} - \frac{1}{n} \right) \right] E \left[ \left( \frac{N_j}{m} - \frac{1}{n} \right) \right] \right) - \hat{Y}(\hat{F})^2 \lambda \eta \text{Var} \left( \frac{N_i}{m} - \frac{1}{n} \right)
\]

\[
= \frac{\hat{Y}(\hat{F})^2 mn(mn^2)}{5} \left( \frac{1}{mn^2} (2 - \frac{1}{mn^2}) + \frac{1}{mn^2} \right) - \frac{\hat{Y}(\hat{F})^2 mn^2}{5} \left( \frac{1}{mn^2} \right) \left( \frac{1}{mn^2} - \frac{1}{mn^2} \right)
\]

\[
= \frac{\hat{Y}(\hat{F})^2}{5} \left( 2 + mn - n + mn^2 + \frac{6}{mn} - \frac{6}{mn^2} + \frac{4}{n^3} \right)
\]

A.3. Proof of Theorem 3

Proof.

\[
\text{Var} \left( W_r(\hat{F}_{b1}) \right) = \text{Var} \left( \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r \left( \hat{F}_{b1,b2}^{**} \right) - \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r \left( \hat{F}_{b1,b2}^{*} \right) \right)
\]

\[
= \text{Var} \left( \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r \left( \hat{F}_{b1,b2}^{**} \right) \right) + \text{Var} \left( \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r \left( \hat{F}_{b1,b2}^{*} \right) \right)
\]

\[
- 2 \text{Cov} \left( \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r \left( \hat{F}_{b1,b2}^{**} \right), \frac{1}{B_2} \sum_{b_2=1}^{B_2} Y_r \left( \hat{F}_{b1,b2}^{*} \right) \right)
\]

\[
= \frac{\text{Var} \left( Y_r \left( \hat{F}_{b1,b2}^{**} \right) \right)}{B_2} + \frac{B_2 - 1}{B_2} \text{Cov} \left( Y_r \left( \hat{F}_{b1,b2}^{**} \right), Y_r \left( \hat{F}_{b1,b2}^{*} \right) \right)
\]

\[
+ \frac{\text{Var} \left( Y_r \left( \hat{F}_{b1,b2}^{**} \right) \right)}{B_2} + \frac{B_2 - 1}{B_2} \text{Cov} \left( Y_r \left( \hat{F}_{b1,b2}^{*} \right), Y_r \left( \hat{F}_{b1,b2}^{**} \right) \right)
\]

\[
- \frac{2}{B_2^2} B_2^2 \text{Cov} \left( Y_r \left( \hat{F}_{b1,b2}^{**} \right), Y_r \left( \hat{F}_{b1,b2}^{*} \right) \right).
\]

As proved in [DeGroot 1989], the variance and covariance between averages of bootstrap samples can be calculated as a function of the variance of the random variable, which for our case is, for a
given \( r \), \( \text{Var} \left( Y_r(\hat{F}_{b_1}^*) \right) \). Since we are looking at the conditional variance, \( \text{Var} \left( Y_r(\hat{F}_{b_1}^*) \right) \) is no longer random (for brevity we refer to \( \text{Var} \left( Y_r(\hat{F}_{b_1}^*) \right) \) as \( \sigma^2 \)). Therefore,

\[
\text{Var} \left( W_r(\hat{F}_{b_1}^*) \right) = \frac{\sigma^2(2m^* - 1)}{B_2(m^*)^2} \left( 1 + \frac{1}{B_2} \right) + \frac{(B_2 - 1)\sigma^2}{B_2m^*} \left( 1 + \frac{B_2 - 1}{B_2} \right) - 2\frac{\sigma^2}{m^*}.
\]

Setting the variance of the bias to be in the order of \( \Theta \left( \text{Var} \left( Y \left( \hat{F}_{b_1}^* \right) \right) / (m^*)^3 \right) \) results in

\[
B_2^* = \Theta \left( \left( \frac{3(m^*)^2 - m^*}{m^* + 1} \right)^{1/3} \right).
\]

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