Data Banzhaf: A Data Valuation Framework with Maximal Robustness to Learning Stochasticity

Tianhao Wang¹ and Ruoxi Jia²

¹Princeton University
²Virginia Tech

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Abstract

This paper studies the robustness of data valuation to noisy model performance scores. Particularly, we find that the inherent randomness of the widely used stochastic gradient descent can cause existing data value notions (e.g., the Shapley value and the Leave-one-out error) to produce inconsistent data value rankings across different runs. To address this challenge, we first pose a formal framework within which one can measure the robustness of a data value notion. We show that the Banzhaf value, a value notion originated from cooperative game theory literature, achieves the maximal robustness among all semivalues—a class of value notions that satisfy crucial properties entailed by ML applications. We propose an algorithm to efficiently estimate the Banzhaf value based on the Maximum Sample Reuse (MSR) principle. We derive the lower bound sample complexity for Banzhaf value estimation, and we show that our MSR algorithm’s sample complexity is close to the lower bound. Our evaluation demonstrates that the Banzhaf value outperforms the existing semivalue-based data value notions on several downstream ML tasks such as learning with weighted samples and noisy label detection. Overall, our study suggests that when the underlying ML algorithm is stochastic, the Banzhaf value is a promising alternative to the semivalue-based data value schemes given its computational advantage and ability to robustly differentiate data quality.

1 Introduction

Data valuation aims at quantifying the usefulness of each data source for machine learning (ML) tasks. It can empower a broad variety of applications. For instance, measuring data value allows data analysts to filter out poor quality data and identify data sources that are important to collect in the future [Jia et al., 2019c, Ghorbani and Zou, 2019, Wang et al., 2020, 2021]. Moreover, it informs the implementation of policies that enable individuals to control how their data is used and monetized by third parties [Voigt and Von dem Bussche, 2017].

Recently, there has been a surge of research efforts on formalizing the notion of data value for supervised ML [Jia et al., 2019b,a, Ghorbani and Zou, 2019, Yan and Procaccia, 2020, Ghorbani et al., 2021, Kwon and Zou, 2021, Yoon et al., 2020]. In the ML context, the value of one data point depends on the other points used in tandem to train a model. For instance, adding extra data points that are similar to an existing data point into the training set decreases the value of the existing one. To accommodate this interplay, data valuation for ML typically starts by defining the “utility” of a
set of data points and then measures the value of an *individual* point based on the change of utility when the point is added to a set of other points. For ML tasks, the utility of a dataset is naturally chosen to be the performance score (e.g., test accuracy) of a model trained on the dataset. Data value notions are computed based on these performance scores, through specific algorithms.

However, stochastic training methods such as stochastic gradient descent (SGD) are widely adopted in ML, especially for deep learning. The models trained with stochastic methods are essentially random and so are their performance scores. This in turn makes the data values calculated from the performance scores *noisy*. We find that despite being ignored in the past, the noise in a typical learning process is actually substantial enough to make different runs of data valuation algorithm produce inconsistent value rankings. Such inconsistency can pose challenges for building reliable applications based upon the data valuation results, e.g., data subset selection and low-quality data identification.

In this paper, we study the robustness of data valuation to noisy model performance scores. Our technical contributions are listed as follows.

**Banzhaf value: a value notion with maximal robustness.** We start by formalizing what it means mathematically for a data value notion to be robust. We introduce the concept of *safety margin*, which is the norm of the largest perturbation of model performance scores that can be tolerated so that the value order of every pair of data points remains unchanged. We prove that the Banzhaf value [Banzhaf III, 1964], a classic value notion from cooperative game theory that was proposed more than half a century ago, achieves the largest safety margin among all semivalues—a class of value notions that satisfy *linearity, dummy player, and symmetry* properties (the LOO error and the Shapley value are special instances of it). Particularly, the safety margin of the Banzhaf value is exponentially larger than that of the Shapley and LOO error.

**Efficient Banzhaf value estimation algorithm.** Similar to Shapley value, Banzhaf value is also costly in computation. We present an efficient Banzhaf value estimation algorithm based on the principle of Maximum Sample Reuse (MSR). We show that our MSR estimation algorithm achieves sizable savings in sample complexity compared with simple Monte Carlo method. We also show that the existence of an efficient MSR estimator is *unique* for the Banzhaf value among all existing semivalue-based data value notions. Moreover, we derive a lower bound of sample complexity for the Banzhaf value estimation, and we show that our MSR estimator’s sample complexity is *close to* matches this lower bound. Additionally, we show that the MSR estimator is robust against the noise in performance scores.

**Experiments.** In the experiment, we demonstrate the ability of Banzhaf value in preserving value rankings with respect to noisy model performance scores. We also demonstrate the sample efficiency of MSR estimator for Banzhaf value. We then show that the Banzhaf value outperforms the state-of-the-art semivalue-based data value notions (including the Shapley value, the LOO error, and the recently proposed Beta Shapley [Kwon and Zou, 2021]) on several downstream ML tasks including bad data detection and data reweighting, where the target model architectures are deep neural networks.

We call the suite of our data value notion and the associated estimation algorithm, the *Data Banzhaf* framework. Overall, our work suggests that Data Banzhaf is a promising alternative to the existing semivalue-based data value notions given its computational advantage and the ability to robustly distinguish data quality in the presence of learning stochasticity.
2 Background: From Leave-One-Out to Shapley to Semivalue

In this section, we formalize the data valuation problem for ML. Then, we review the the concept of LOO and Shapley value—the most popular data value notions in the existing literature, as well as semivalues, which are recently introduced as a natural relaxation of Shapley value in ML context.

**Data valuation problem set-up.** Let $N = \{1, \ldots, n\}$ denotes a training set of size $n$. The objective of data valuation is to assign a score to each training data point in a way that respects the constraints (i.e., axioms) naturally entailed by the applications of the scores. We will refer to these scores as *data values*. For instance, if one would use the scores to design incentives for collaborative learning, then the scores need to fairly reflect the contribution of individual data points to the learning task. To analyze a point’s “contribution”, we define a *utility function* $U : 2^N \to \mathbb{R}$, which maps any subset of the training set to a score indicating the usefulness of the subset. $2^N$ represents the power set of $N$, i.e., the set of all subsets of $N$, including the empty set and $N$ itself. For classification task, a common choice for $U$ is the validation accuracy of a model trained on the input subset. Formally, we have $U(S) = \text{acc}(A(S))$, where $A$ is a learning algorithm that takes a dataset $S$ as input and returns a model, and $\text{acc}$ is a metric function to evaluate the performance of a given model, e.g., the accuracy of a model on a hold-out test set. Without loss of generality, we assume throughout the paper that $U(S) \in [0,1]$. For notation simplicity, we sometimes denote $S \cup i = S \cup \{i\}$ and $S \backslash i = S \backslash \{i\}$ for singleton $\{i\}$, where $i \in N$ represents a single data point.

**LOO Error.** A simple data value measure is leave-one-out (LOO) error, which calculates the change of model performance when the data point $i$ is excluded from the training set $N$:

$$\phi_{\text{loo}}(i; U) := U(N) - U(N \backslash i)$$

(1)

However, many empirical studies [Ghorbani and Zou, 2019, Jia et al., 2019c] suggest that it underperforms other alternatives in differentiating data quality.

**Shapley Value.** The Shapley value is arguably the most widely studied scheme for data valuation. At a high level, it appraises each point based on the (weighted) average utility change caused by adding the point into different subsets. The Shapley value of a data point $i$ is defined as

$$\phi_{\text{shap}}(i; U) := \frac{1}{n} \sum_{k=1}^{n} \binom{n-1}{k-1} \sum_{S \subseteq N \backslash \{i\}, |S| = k-1} [U(S \cup i) - U(S)]$$

(2)

The popularity of the Shapley value is attributable to the fact that it is the only data value notion satisfying the following four axioms [Shapley, 1953]:

- **Dummy player:** if $U(S \cup i) = U(S) + c$ for all $S \subseteq N \backslash i$ and some $c \in \mathbb{R}$, then $\phi(i; U) = c$.
- **Symmetry:** if $U(S \cup i) = U(S \cup j)$ for all $S \subseteq N \backslash \{i, j\}$, then $\phi(i; U) = \phi(j; U)$.
- **Linearity:** For utility functions $U_1, U_2$ and any $\alpha_1, \alpha_2 \in \mathbb{R}$, $\phi(i; \alpha_1 U_1 + \alpha_2 U_2) = \alpha_1 \phi(i; U_1) + \alpha_2 \phi(i; U_2)$.
- **Efficiency:** for every $U, \sum_{i \in N} \phi(i; U) = U(N)$.

$U(S \cup i) - U(S)$ is often termed the *marginal contribution* of data point $i$ to subset $S \subseteq N \backslash i$. We refer the readers to [Jia et al., 2019b, Ghorbani and Zou, 2019] for a detailed discussion about the interpretation of dummy player, symmetry, and linearity axioms in ML. The efficiency axiom, however, receives more controversy than the other three. The *efficiency* axiom requires the total sum of data values to be equal to the utility of full dataset $U(N)$. Recent work [Kwon and Zou,
argues that this axiom is considered not essential in ML. Firstly, the choice of utility function in the ML context is often not directly related to monetary value so it is unnecessary to ensure the sum of data values matches the total utility. Moreover, many applications of data valuation, such as bad data detection, are performed based only on the ranking of data values. For instance, multiplying the Shapley value by a positive constant does not affect the order of the data values. Hence, there are many data values that do not satisfy the efficiency axiom, but can still be used for differentiating data quality, just like the Shapley value.

**Semivalue.** The class of data values that satisfy all the Shapley axioms except efficiency is called *semivalues*. It was originally studied in the field of economics and recently proposed to tackle the data valuation problem [Kwon and Zou, 2021]. Unlike the Shapley value, semivalues are not unique. The following theorem by the seminal work of [Dubey et al., 1981] shows that every semivalue of a data point $i$ can be expressed as the weighted average of marginal contributions $U(S \cup i) - U(S)$ across different subsets $S \subseteq N \setminus i$.

\[ \phi_{\text{semi}}(i; U, w) := \frac{1}{n} \sum_{k=1}^{n} w(k) \sum_{S \subseteq N \setminus \{i\}, |S| = k-1} [U(S \cup i) - U(S)] \]  

Note that semivalues can subsume both the Shapley value and the LOO error with $w(k) = \binom{n-1}{k-1}$ and $w(k) = n1[k = n]$, respectively. Despite its theoretical attraction, the question remains which one of the many semivalues we should adopt.

### 3 Utility Function Can Be Stochastic

In this section, we will delve into the stochasticity of the utility function, which is prevalent for modern ML models but largely overlooked in the prior work. We show that it can cause significant instability in data value estimation. This section serves as a motivation to investigate the semivalues with maximal robustness.

In the existing literature, the utility of a dataset $U(S)$ is often defined to be $\text{acc}(\mathcal{A}(S))$, i.e., the performance of a model $\mathcal{A}(S)$ trained on a dataset $S$. However, many learning algorithms $\mathcal{A}$ such as SGD contains randomness. Since the loss function for training neural networks is non-convex, the trained model greatly depends on the randomness of the training process, e.g., random mini-batch selection. Thus, $U(S)$ defined in this way in turn becomes a randomized function.
Signal-to-noise ratio of marginal contribution. As the data values are calculated through the marginal contributions of individual points, we first investigate the impact of learning stochasticity on the reliability of marginal contribution estimates. To do so, we randomly pick a pair of $i \in N$ and $S \in N \setminus i$, train 50 models on each of $S \cup i$ and $S$, and use the signal-to-noise ratio (SNR) $\frac{E[|acc(A(S)) - acc(A(S\cup i))|]}{Std(acc(A(S\cup i)) - acc(A(S)))}$ to measure the reliability of marginal contribution estimates, where $Std$ denotes the standard deviation. Figure 1 shows an example of the estimated SNR of marginal contribution with different architectures and training hyperparameters on the MNIST dataset. As we can see, the SNR of marginal contribution is very low (near 0.1) for most of the settings. In particular, $SNR$ is consistently low regardless of the cardinality of $S$. When $|S|$ is small, while the contribution of an additional data point $i$ may be significant, the performance variance of the trained model may be large due to the small training size. When $|S|$ is large, while performance variance is small, the contribution of an additional data point $i$ becomes insubstantial.

Instability of data value rankings. Semivalues are calculated by taking a weighted average of marginal contributions. When the weights are not properly chosen, the noisy estimate of marginal contributions can cause significant instability in ranking the data values. Figure 2 (a)-(b) illustrates the estimates of two popular data value notions—LOO error and the Shapley value—on 20 different data points, when the utility function is the accuracy of a neural network trained via SGD. The experiment settings are detailed in Appendix C.2. As we can see, the variance of the data value estimates caused by learning stochasticity outweighs their magnitude for both notions. As a result, the rankings of data values across different runs are largely inconsistent (e.g., the average Spearman coefficient of Shapley rankings across different runs is 0.06). Leveraging the rankings of such data values to differentiate data quality can be unreliable, as evidenced in the Evaluation Section.

Redefine $U$ as expected performance. To make the data value notions independent of the learning stochasticity, we can redefine $U$ to be $U(S) = E_{\mathcal{A}}[acc(A(S))]$, the expected performance of the trained model. However, accurately estimating $U(S)$ under this new definition requires running $\mathcal{A}$ multiple times on the same $S$, and calculating the average utility of $S$. Obviously, this simple approach incurs a large extra computational cost. On the other hand, if we estimate $U(S)$ with only one or few calls of $A$, the estimate of $U(S)$ will be very noisy, resulting in unreliable data value estimates as we have shown above. Hence, we pose the question: is it possible to obtain robust data value estimates without naively investing more computation?
4 Data Banzhaf: A Framework for Robust Data Valuation

To address the question posed above, this section starts by formalizing the notion of robustness in data valuation. Then, we show that the most robust semivalue, surprisingly, coincides with the Banzhaf value [Banzhaf III, 1964]—a famous value assignment scheme in cooperative game theory. We also develop algorithms to enable efficient estimation of the Banzhaf value.

4.1 Ranking Stability as a Robustness Notion

In many applications of data valuation such as data selection, it is the order of data values that matters [Kwon and Zou, 2021]. For instance, to filter out low-quality data, one would first rank the data points based on their values and then throw the points with the lowest values. When the utility functions are perturbed by noise, we would like the rankings of the data values to remain stable. Recall that a semivalue is defined by a weight function \( w \) such that \( \sum_{k=1}^{n} \frac{(n-1)}{k-1} w(k) = n \). The (scaled) difference between the semivalues of two data points \( i \) and \( j \) can be easily computed from expression (3):

\[
D_{i,j}(U; w) := n(\phi(i; w) - \phi(j; w)) = \sum_{k=1}^{n-1} (w(k) + w(k+1)) \left( \frac{n-2}{k-1} \right) \Delta_{i,j}^{(k)}(U)
\]

where \( \Delta_{i,j}^{(k)}(U) = \left( \frac{n-2}{k-1} \right)^{-1} \sum_{|S| = k-1, \ S \subseteq N \setminus \{i, j\}} [U(S \cup i) - U(S \cup j)] \). This quantity considers all possible \( S \in N \setminus \{i, j\} \) with the same cardinality and measures the average difference of \( U \) when datum \( i \) is replaced by \( j \). \( \Delta_{i,j}^{(k)}(U) \) represents the average distinguishability between \( i \) and \( j \) on size-\( k \) sets using the noiseless utility function \( U \).

Let \( \hat{U} \) denote a noisy estimate of \( U \). \( \hat{U} \) and \( U \) produce different data value orders for \( i, j \) if and only if \( D_{i,j}(U; w)D_{i,j}(\hat{U}; w) \leq 0 \). However, if the noiseless \( U \) itself cannot sufficiently differentiate between \( i \) and \( j \) on sets of all sizes (i.e., \( \Delta_{i,j}^{(k)}(U) \approx 0 \) for \( k = 1, \ldots, n-1 \)), then \( D_{i,j}(U; w) \) will be (nearly) zero and infinitesimal perturbation can switch the ranking of \( \phi(i) \) and \( \phi(j) \). To reasonably define the robustness of semivalues, we need to only consider the utility functions who can sufficiently “distinguish” between \( i \) and \( j \).

**Definition 2.** We say a data point pair \( (i, j) \) is \( \tau \)-distinguishable by \( U \) if and only if \( \Delta_{i,j}^{(k)}(U) \geq \tau \) for all \( k \in \{1, \ldots, n-1\} \).

Let \( \mathcal{U}_{i,j}^{(\tau)} \) denote the collection of utility functions \( U \) that can \( \tau \)-distinguish a pair \( (i, j) \). With the definition of distinguishability, we can characterize the robustness of a semivalue by computing its “safety margin”, which is the minimum amount of perturbation \( \|\hat{U} - U\| \) needed to reverse the ranking of at least one pair of data points \( (i, j) \), for at least one utility function \( U \) from \( \mathcal{U}_{i,j}^{(\tau)} \).

**Definition 3 (Safety margin).** Given \( \tau > 0 \), we define the safety margin of a semivalue as

\[
\text{Safe}(\tau; w) = \min_{i,j \in N, i \neq j} \min_{U \in \mathcal{U}_{i,j}^{(\tau)}} \min_{\hat{U} \in \{\hat{U}: D_{i,j}(U; w)D_{i,j}(\hat{U}; w) \leq 0\}} \|\hat{U} - U\|
\]

The safety margin captures the largest noise that can be tolerated by a semivalue without altering the ranking of any pair of data points that are distinguishable by the original utility function. In
Appendix, we show that the LOO and Shapley value’s safety margin is bounded by \( \tau \) and \( \tau(n-1) \), respectively. We find that, Banzhaf value, which is the simple average of the marginal contribution of a data point against all subsets, achieves the largest safety margin among all semivalues. We first recall the Banzhaf value, a classic value notion for profit sharing from cooperative game theory.

**Definition 4 ([Banzhaf III, 1964])**. The Banzhaf value for data point \( i \) is defined as

\[
\phi_{\text{banz}}(i; U, N) := \frac{1}{2^{n-1}} \sum_{S \subseteq N \setminus i} [U(S \cup i) - U(S)]
\]

The Banzhaf value is a semivalue, as we can recover its definition (6) from the general expression of semivalues (3) by setting constant weight function \( w(k) = \frac{n}{2^{n-1}} \) for all \( k \in \{1, \ldots, n\} \).

**Theorem 5.** For any \( \tau > 0 \), Banzhaf value \( (w(k) = \frac{n}{2^{n-1}}) \) achieves the largest safety margin \( \text{Safe}(\tau; w) = \tau 2^{n/2-1} \) among all semivalues.

The intuition for the superior robustness of the Banzhaf value can be explained as follows: Semivalues assign different weights to the marginal contribution against different data subsets according to the weight function \( w \). To construct a perturbation of the utility function that maximizes the influence on the corresponding semivalue, one needs to perturb the utility of the subsets that are assigned with higher weights. Hence, the best robustification strategy is to assign uniform weights to all subsets, which leads to the Banzhaf value. On the other hand, semivalues that assign heterogeneous weights to different subsets, such as Shapley and LOO error, suffer a lower safety margin.

One can also show that Banzhaf value is most robust in the sense that the utility noise will minimally affect data value changes. Or in other words, the Banzhaf value achieves the smallest Lipschitz constant \( L \) such that \( \|\phi(U) - \phi(\hat{U})\| \leq L\|U - \hat{U}\| \) for all possible pairs of \( U \) and \( \hat{U} \). We refer the reviewer to Appendix B.6 for details. This result shows that Data Banzhaf is also the most robust semivalue in minimizing the change of data value magnitude.

### 4.2 Efficient Banzhaf Value Estimation

Similar to the Shapley value and the other semivalue-based data value notions, the exact computation of the Banzhaf value can be expensive because it requires an exponential number of utility function evaluations, which entails an exponential number of model fittings. This could be a major challenge for adopting the Banzhaf value in practice. To address this issue, we present a novel Monte Carlo algorithm to approximate the Banzhaf value.

We start by defining the estimation error of a semivalue estimator. We say a semivalue estimator \( \hat{\phi} \) is an \((\epsilon, \delta)\)-approximation to the true semivalue \( \phi \) (in \( \ell_p \)-norm) if and only if \( \Pr_{\hat{\phi}}[\|\phi - \hat{\phi}\|_p \leq \epsilon] \geq 1 - \delta \) where the randomness is over the execution of the estimator. For any data point pair \((i, j)\), if \( |\phi(i) - \phi(j)| \geq 2\epsilon \), then an estimator that is \((\epsilon, \delta)\)-approximation in \( \ell_\infty \)-norm is guaranteed to keep the data value order of \( i \) and \( j \) with probability at least \( 1 - \delta \).

**Baseline: Simple Monte Carlo.** The Banzhaf value can be equivalently expressed as follows:

\[
\phi_{\text{banz}}(i) = \mathbb{E}_{S \sim \text{Unif}(2^{N\setminus i})} [U(S \cup \{i\}) - U(S)]
\]

where \( \text{Unif}(\cdot) \) to denote Uniform distribution over the power set of \( N \setminus \{i\} \). Thus, a straightforward Monte Carlo (MC) method to estimate \( \phi_{\text{banz}}(i) \) is to sample a collection of data subsets \( S_i \) from
$2^N \cdot$ uniformly at random, and then compute $\hat{\phi}_{MC}(i) = \frac{1}{|S_i|} \sum_{S \in S_i} (U(S \cup i) - U(S))$. We can repeat the above procedure for each $i \in N$ and obtain the approximated semivalue vector $\hat{\phi}_{MC} = [\hat{\phi}_{MC}(1), \ldots, \hat{\phi}_{MC}(n)]$. Since $U(S \cup i) - U(S)$ is a bounded random variable, we can obtain the sample complexity of this simple MC estimator by the Hoeffding’s inequality.

**Theorem 6** ([Bachrach et al., 2010]). $\hat{\phi}_{MC}$ is an $(\varepsilon, \delta)$-approximation to the exact Banzhaf value in $\ell_2$-norm with $O\left(\frac{n^2}{\varepsilon^2} \log\left(\frac{\eta}{\delta}\right)\right)$ calls of $U(\cdot)$, and in $\ell_\infty$-norm with $O\left(\frac{n^4}{\varepsilon^2} \log\left(\frac{\eta}{\delta}\right)\right)$ calls of $U(\cdot)$.

**Proposed Algorithm: Maximum Sample Reuse (MSR) Monte Carlo.** The simple MC method is sub-optimal since, for each sampled $S \in S_i$, the value of $U(S)$ and $U(S \cup i)$ are only used for estimating $\phi_{banz}(i)$, i.e., the Banzhaf value of a single datum $i$. This inevitably results in a factor of $n$ in the final sample complexity as we need the same amount of samples to estimate each $i \in N$. To address this weakness, we propose an advanced MC estimator which achieves maximum sample reuse (MSR). Specifically, by the linearity of expectation, we have $\phi_{banz}(i) = E_{S \sim \text{Unif}(2^N \setminus i)} [U(S \cup i)] - E_{S \sim \text{Unif}(2^N \setminus i)} [U(S)]$. Suppose we have $m$ samples $S = \{S_1, \ldots, S_m\}$ i.i.d. drawn from $\text{Unif}(2^N)$. For every data point $i$ we can divide $S$ into $S_{2i} \cup S_{2i}^c$, where $S_{2i} = \{S \in S : i \in S\}$ and $S_{2i}^c = \{S \in S : i \notin S\} = S \setminus S_{2i}$. We can then estimate $\phi(i)$ by

$$\hat{\phi}_{MSR}(i) = \frac{1}{|S_{2i}|} \sum_{S \in S_{2i}} U(S) - \frac{1}{|S_{2i}^c|} \sum_{S \in S_{2i}^c} U(S)$$

(8)

or set $\hat{\phi}_{MSR}(i) = 0$ if either of $|S_{2i}|$ and $|S_{2i}^c|$ is 0. In this way, every evaluation of $U(S)$ is used in the estimation of $\phi(i)$ for all $i \in N$. We will call this new estimator the MSR estimator.

**Theorem 7.** $\hat{\phi}_{MSR}$ is an $(\varepsilon, \delta)$-approximation to the exact Banzhaf value in $\ell_2$-norm with $O\left(\frac{n^2}{\varepsilon^2} \log\left(\frac{\eta}{\delta}\right)\right)$ calls of $U(\cdot)$, and in $\ell_\infty$-norm with $O\left(\frac{n^4}{\varepsilon^2} \log\left(\frac{\eta}{\delta}\right)\right)$ calls of $U(\cdot)$.

Compared with Simple MC method, the MSR estimator saves a factor of $n$ in the sample complexity. We remark that this sample complexity is non-trivial to derive. Unlike the simple Monte Carlo, the sizes of the samples that we average over in (8) (i.e., $|S_{2i}|$ and $|S_{2i}^c|$) are also random variables. Hence, we cannot simply apply the Hoeffding’s inequality to get a high-probability bound for $|\hat{\phi}_{MSR} - \phi_{banz}|$. The key to the proof is to notice that $|S_{2i}|$ follows binomial distribution $\text{Bin}(m, 0.5)$. Thus, we first show that $|S_{2i}|$ is close to $m/2$ with high probability and then apply the Hoeffding’s inequality to bound the difference between $\frac{1}{m/2} \sum_{S \in S_{2i}} U(S) - \frac{1}{m/2} \sum_{S \in S_{2i}^c} U(S)$ and $\phi_{banz}(i)$.

**Can estimation of other semivalues with MSR enjoy similar efficiency gains?** Every semivalue can be written as the expectation of weighted marginal contribution $\phi_{semi}(i; U, N, w) = \frac{2^{n-1}}{n} \left( E_{S \sim \text{Unif}(\{S \in 2^N : \exists i \in S\})} [w(|S|)U(S)] - E_{S \sim \text{Unif}(2^N \setminus i)} [w(|S| + 1)U(S)] \right)$. Hence, one could construct an MSR estimator for arbitrary semivalue as follows: $\hat{\phi}_{MSR}(i) = \frac{2^{n-1}}{m|S_{2i}|} \sum_{S \in S_{2i}} w(|S|)U(S) - \frac{2^{n-1}}{m|S_{2i}^c|} \sum_{S \in S_{2i}^c} w(|S| + 1)U(S)$. For the Shapley value, $w(|S|) = \binom{n}{|S|-1}^{-1}$. This combinatorial coefficient makes the calculation of this estimator numerically unstable when $n$ is large. As we will show in the Appendix B.2, it turns out that it is also impossible to construct a distribution $\mathcal{D}$ over $2^N$ s.t. $\phi_{shap}(i) = E_{S \sim \mathcal{D} \cup \{i\}} [U(S)] - E_{S \sim \mathcal{D} \setminus \{i\}} [U(S)]$ for the Shapley value and any other data value notions except the Banzhaf value. Therefore, the existence of the efficient MSR estimator is a unique advantage of the Banzhaf value.

We note that the Group Testing-based estimator from [Jia et al., 2019b] for Shapley value also achieves $O\left(\frac{n^2}{\varepsilon^2} \log\left(\frac{\eta}{\delta}\right)\right)$ sample complexity in $\ell_2$-norm asymptotically. The key idea is to estimate $\phi_{shap}(i)$ for a fixed $i$ and $\phi_{shap}(i) - \phi_{shap}(j)$ for every $j \neq i$. In Appendix B.3, we introduce an
improved Group Testing-based Shapley estimator. However, as we will show in the evaluation section, even with the improved version of Group Testing estimator, the estimated Shapley value converges more slowly than both simple MC and MSR estimators of the Banzhaf value in terms of value rankings.

**Lower Bound for Banzhaf Value Estimation.** To understand the optimality of the MSR estimator, we derive a lower bound for any Banzhaf estimator that achieves $(\varepsilon, \delta)$-approximation in $\ell_\infty$-norm.

**Theorem 8.** Every (randomized) Banzhaf value estimator that achieves $(\varepsilon, \delta)$-approximation in $\ell_\infty$-norm for constant $\delta \in (0, 1/2)$ has sample complexity at least $\Omega(\frac{1}{\varepsilon})$.

Recall that our MSR algorithm achieves $\tilde{O}(\frac{1}{\varepsilon^2})$ sample complexity. This means that our MSR algorithm is close to optimal, as there is only an extra factor of $\frac{1}{\varepsilon}$. The main idea of deriving the lower bound is to use Yao’s minimax principle. Specifically, we construct a distribution over instances of utility functions and prove that no deterministic algorithm can work well against that distribution.

**Robustness of MSR Estimator Under Noisy Utility Function.** As discussed in Section 3, the utility function $U$ is re-defined as the expected model performance due to the stochasticity of the underlying learning algorithm. Hence, the actual estimator of the Banzhaf value that we build is based upon the noisy variant $\tilde{U}$:

$$\tilde{\phi}_{\text{MSR}}(i) = \frac{1}{|S \ni i|} \sum_{S \ni i} \tilde{U}(S) - \frac{1}{|S \ni i|} \sum_{S \ni i} \tilde{U}(S).$$

(9)

Hence, it is interesting to understand the impact of noisy utility function evaluation on the sample complexity of the MSR estimator.

**Theorem 9.** When $\|U - \tilde{U}\|_2 \leq \gamma$, $\tilde{\phi}_{\text{MSR}}$ is $(\varepsilon + \frac{\gamma \sqrt{n}}{2n^{1/2}}, \delta)$-approximation in $\ell_2$-norm with $O(\frac{n}{\varepsilon^2} \log \frac{n}{\delta})$ calls, and $(\varepsilon + \frac{\gamma}{2n^{1/2}}, \delta)$-approximation in $\ell_\infty$-norm with $O(\frac{1}{\varepsilon^2} \log \frac{n}{\delta})$ calls to $\tilde{U}$.

The theorem above shows that our MSR algorithm has the same sample complexity in the presence of noise in $\tilde{U}$, with a small extra irreducible error since typically $\gamma \propto \sqrt{2^n} = 2^{n/2}$.

## 5 Evaluation

Our evaluation covers the following aspects: (1) Sample efficiency of the proposed MSR estimator for the Banzhaf value; (2) Robustness of the Banzhaf value compared to the six existing semivalue-based data value notions (including Shapley value, LOO error, and four representatives from Beta Shapley$^3$); (3) Effectiveness of performing noisy label detection and learning with weighted samples based on the Banzhaf value. Detailed settings are provided in Appendix C.3, C.4, and C.5.

### 5.1 Sample Efficiency

**MSR vs. Simple MC.** We compare the sample complexity of the MSR and the simple MC estimator for approximating the Banzhaf value. In order to exactly evaluate the estimation error of the two estimators, we use a synthetic dataset generated by multivariate Gaussian with only 10 data points—a scale where we can compute the Banzhaf value exactly. The utility function is the

$^3$We evaluate Beta(1, 4), Beta(1, 16), Beta(4, 1), Beta(16, 1) as the original paper.
validation accuracy of logistic regression trained with full-batch gradient descent; thus, there is no randomness in training. The randomness associated with the estimator error is solely from random sampling in the estimation algorithm. Figure 3 (a) compares the variance of the two estimators as the number of samples grows. As we can see, the estimation error of the MSR estimator reduces much more quickly than that of the simple MC estimator. Furthermore, given the same amount of samples, the MSR estimator exhibits a much smaller variance across different runs compared to the simple MC method.

Banzhaf vs. Shapley. We compare Banzhaf value estimators with two popular Shapley value estimators, the Permutation Sampling [Castro et al., 2009] and our improved version of Group Testing algorithm (see the full algorithm in Appendix B.3). Since the Shapley and Banzhaf values are of different scales, for a fair comparison, we measure the consistency of the order of estimated data values. Specifically, we increase the sample size by adding a new batch of samples at every iteration and evaluate each of the estimators on different sample sizes. For each estimator, we calculate the relative Spearman index, which is the Spearman index of the value estimates between two adjacent iterations. A high Relative Spearman Index means the ranking does not change too much with extra samples, which implies convergence of data value rankings. Figure 3 (b) compares the relative spearman index of different data value estimators when the utility functions are defined as a small CNN trained on MNIST dataset. We can see that the MSR estimator for the Banzhaf value converges much faster than the two estimators for Shapley value in terms of the ranking of data values.

5.2 Ranking Preservation under Noisy Utility Functions

We compare the robustness of different data value notions in preserving the ranking of data values against the utility score perturbation due to the stochasticity in SGD. The tricky part in the experiment design is that we need to adjust the scale of the perturbation caused by natural stochastic learning algorithm. In Appendix C.5, we show a procedure for controlling the magnitude of perturbation with a single parameter $k$: the larger the $k$, the smaller the noise magnitude. In Figure 4 (a), we plot the Spearman index between the ranking of reference data values and the ranking of data values computed from noisy utility scores. Specific experiment settings are deferred to the Appendix C.5. As we can see, Data Banzhaf achieves the most stable ranking and its stability advantage gets more prominent as the noise increases. Moreover, we show the box-plot of Banzhaf value estimates in Figure 2 (c) evaluated on the MNIST dataset. Compared with Shapley and LOO,
Table 1: Accuracy comparison of models trained with weighted samples. We compare the seven data valuation methods on the 13 classification datasets. The average and standard error of classification accuracy are denoted by ‘average (standard error)’. The standard error is only due to the stochasticity in utility function evaluation. Boldface numbers denote the best method. Beta Shapley does NOT applicable for datasets with \( \geq 1000 \) data points (MNIST, FMNIST, CIFAR10, and Click) due to numerical issue. ‘Uniform’ denotes training with uniformly weighted samples.


classification learning stochasticity has a much smaller impact on the ranking of Banzhaf values.

5.3 Applications of Data Banzhaf

Given the promising results obtained from the proof-of-concept evaluation on synthetic datasets, we move forward to real-world datasets and evaluate the effectiveness of Data Banzhaf in distinguishing data quality for machine learning tasks. Particularly, we considered two applications enabled by data valuation: one is to reweight training data during learning and another is to detect mislabeled points. We use neural networks trained with Adam as the learning algorithm wherein the associated utility function is noisy in nature. We compare with 6 baselines that are previously proposed semivalue-based data value notions: Data Shapley, Leave-one-out (LOO), and 4 variations of Beta Shapley proposed in [Kwon and Zou, 2021] (Beta(1, 4), Beta(1, 16), Beta(4, 1), Beta(16, 1)). We use 13 standard datasets that are previously used in the data valuation literature to benchmark classification methods.

Learning with Weighted Samples. Similar to [Kwon and Zou, 2021], we weight each training point by normalizing the associated data value between [0,1]. Then, during training, each training sample will be selected with a probability equal to the assigned weight. As a result, data points with a higher value are more likely to be selected in the random mini-batch of SGD, and data points with a lower value are rarely used. We train a neural network classifier to minimize the weighted loss, and then evaluate the accuracy on the held-out test dataset. As Table 1 shows, Data Banzhaf outperforms other baselines. To investigate the impact of the noise scale on the quality of different data value notions, we design an experiment where we can control the noise scale. Specifically, we train a logistic regression with gradient descent to minimize the weighted loss. Due to the convexity of logistic regression, the resulting utility score (i.e., accuracy on the held-out set) is deterministic. Then, we add Gaussian noise of different scales to the utility score. Figure 4 (b) shows that, with clean utility scores (noise scale = 0), Data Banzhaf’s performance is not as good as methods like Beta(4, 1) or Beta(16, 1). However, as the noise increases, the performance of all baselines drops significantly while Data Banzhaf maintains a performance similar to the noiseless setting.

Noisy Label Detection. We investigate the ability of different data value notions in detecting mislabeled points under noisy utility functions. We generate noisy labeled samples by flipping labels...
Figure 4: Impact of the noise in utility scores on (a) the Spearman index between the ranking of reference data value and the ranking of data value estimated from noisy utility scores; the larger the $k$, the smaller the noise magnitude., (b) the performance of learning with samples weighted by noisy data values, and (c) the performance of mislabel detection using noisy data values.

| Dataset   | Data Banzhaf | LOO | Beta(1, 16) | Beta(1, 4) | Data Shapley | Beta(4, 1) | Beta(16, 1) |
|-----------|--------------|-----|-------------|-----------|--------------|------------|-------------|
| MNIST     | 0.193 (0.017)| 0.165 (0.009)| -           | -         | 0.135 (0.025)| -          | -           |
| FMNIST    | 0.156 (0.018)| 0.164 (0.014)| -           | -         | 0.135 (0.016)| -          | -           |
| CIFAR10   | **0.22 (0.003)** | 0.086 (0.02)| -           | -         | 0.152 (0.023)| -          | -           |
| Click     | **0.206 (0.01)** | 0.096 (0.034)| -           | -         | 0.116 (0.024)| -          | -           |
| Fraud     | 0.47 (0.024)  | 0.157 (0.046)| 0.14 (0.058)| 0.19 (0.058)| **0.65 (0.032)**| 0.59 (0.037)| 0.55 (0.032)|
| Creditcard| 0.27 (0.024)  | 0.113 (0.073)| 0.17 (0.087)| 0.17 (0.024)| 0.26 (0.049) | **0.28 (0.081)**| 0.25 (0.063)|
| Vehicle   | 0.45 (0.0)    | 0.123 (0.068)| 0.1 (0.055)| 0.16 (0.058)| 0.41 (0.066) | 0.42 (0.068) | 0.43 (0.051)|
| Apsfail   | **0.49 (0.037)** | 0.096 (0.09)| 0.2 (0.071)| 0.22 (0.051)| 0.47 (0.024) | 0.42 (0.024)| 0.36 (0.02)|
| Phoneme   | 0.216 (0.023) | 0.115 (0.026)| 0.088 (0.02)| 0.124 (0.039)| 0.216 (0.032)| **0.236 (0.027)**| 0.232 (0.02)|
| Wind      | 0.36 (0.02)   | 0.073 (0.022)| 0.17 (0.06)| 0.19 (0.086)| **0.57 (0.068)**| 0.52 (0.04) | 0.51 (0.037)|
| Pol       | **0.47 (0.04)** | 0.097 (0.093)| 0.09 (0.02)| 0.17 (0.051)| 0.44 (0.058) | 0.4 (0.055) | 0.26 (0.037)|
| CPU       | 0.35 (0.045)  | 0.107 (0.074)| 0.08 (0.081)| 0.13 (0.068)| 0.46 (0.037) | **0.48 (0.06)** | 0.45 (0.055)|
| 2DPlanes  | **0.52 (0.024)** | 0.136 (0.053)| 0.19 (0.037)| 0.26 (0.073)| 0.51 (0.058) | 0.47 (0.075)| 0.41 (0.058)|

Table 2: Comparison of mislabel data detection ability of the seven data valuation methods on the 13 classification datasets. The average and standard error of F1-score are denoted by ‘average (standard error)’. The standard error is only due to the random noise in the utility function evaluation. Boldface numbers denote the best method in F1-score average.

for a randomly chosen 10% of training data points. We mark a data point as a mislabeled one if its data value is less than 10 percentile of all data value scores. We use F1-score as the performance metric for mislabeling detection. Table 2 in the Appendix shows the F1-score of the 7 data valuation methods and Data Banzhaf shows the best overall performance. Similar to the previous application, we also study the impact of noise scale on detection performance. As Figure 4 (c) shows, the detection performance of all but Data Banzhaf drops as the noise increases.

6 Limitation and Future Work

This work develops Data Banzhaf as a data valuation method that is robust against the perturbation to the utility function, which is common in ML settings. One limitation of Data Banzhaf is the computational challenge. While it allows for a more efficient estimation algorithm compared with Shapley value, an accurate Banzhaf estimation still requires many model retraining, which can be computationally expensive for large model architecture.

There are many interesting future works in this area. During the research, we find that the variance of model performance scores does not have a clear dependency on training hyperparameters such as mini-batch sizes. Exploring the relationship between performance variance and training hyperparameters...
is interesting. Additionally, utility perturbation leads to violation of the axioms satisfied by a semivalue. How to rigorously quantify the degree of violation is also interesting to pursue.
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A Related Work

Cooperative Game Theory-based Data Valuation. Game-theoretic formulations of data valuation have become popular in recent years. Particularly, Shapley value has become a widely accepted data value notion [Ghorbani and Zou, 2019, Jia et al., 2019b,a,c, Wang et al., 2020] as it is the unique value notion which satisfies the four axioms: linearity, dummy player, symmetry, and efficiency. Alternatives to Shapley value for data valuation have also been proposed through the relaxation of the Shapley axioms. Yan and Procaccia [Yan and Procaccia, 2020] propose to use the Least core [Deng and Papadimitriou, 1994], another classic concept in cooperative game theory, as an alternative to the Shapley value for data valuation. At a high level, the Least Core is a profit allocation scheme that requires the smallest subsidy to each coalition $S$ so that no participant has an incentive to deviate from the grand coalition $N$. It is computed by solving the linear programming problem below:

$$\min_{\phi_{LC}} e \quad \text{s.t.} \quad \sum_{i=1}^{n} \phi_{LC}(i) = U(N), \quad \sum_{i \in S} \phi_{LC}(i) + e \geq U(S), \forall S \subseteq N$$  \hspace{1cm} (10)$$

The Least Core defined above satisfies all the Shapley axioms except linearity. By relaxing the efficiency axiom, the class of solution concepts that satisfy linearity, dummy player, and symmetry is called semivalue [Weber, 1988]. Kwon and Zou [Kwon and Zou, 2021] propose Beta Shapley, which is a collection of semivalues that enjoy certain mathematical convenience. However, the construction of Beta Shapley does not take the perturbation of performance scores into account, and the paper only considers deterministic learning algorithm (such as Logistic Regression) in their experiment. In this work, we characterize the Banzhaf value as the most robust semivalue against the perturbation in the performance scores, which is critical for applications involving stochastic training such as neural network training.

Distributional Shapley value [Ghorbani et al., 2020, Kwon et al., 2021] is a variant of Data Shapley which measures the contribution of a data point with respect to a data distribution instead of a static dataset. The stability notion discussed in the paper is in terms of the perturbation to the data point instead of model performance scores. Bian et al. [Bian et al., 2021] take a probabilistic treatment of cooperative games. Through mean-field variational inference in the energy-based model, they develop multiple step Variational Value as a data value notion which satisfies null player, marginalism and symmetry. The marginalism axiom requires a player’s payoffs to depend only on his own marginal contributions – whenever they remain unchanged, his payoffs should be unaffected. Yona et al. [Yona et al., 2021] relax the assumption that the learning algorithm is fixed in advance in the previous work, and extend Shapley value to jointly quantify the contribution of data points and learning algorithms. It improves the stability of data value under domain shifts by attributing the responsibility to the learning algorithm. Agussurja et al. [Agussurja et al., 2022] derive the convergence property of the Shapley value in parametric Bayesian learning games, and apply the result to establish an online collaborative learning framework that is asymptotically Shapley-fair.

Banzhaf Value, Banzhaf power index and friends. What is known today as the Banzhaf value or Banzhaf power index was originally introduced by Lionel Penrose in 1946 [Penrose, 1946]. It was reinvented by John F. Banzhaf III in 1964 [Banzhaf III, 1964], and was reinvented once more by James Samuel Coleman in 1971 [Coleman, 1971] before it became part of the mainstream literature. In the field of machine learning, Banzhaf value has been previously applied to the problem of measuring feature importance [Datta et al., 2015, Kulynych and Troncoso, 2017, Sliwinski et al., 2019, Patel et al., 2021, Karczmarz et al., 2021]. While these works suggest that Banzhaf value...
could be an alternative to the popular Shapley value-based model interpretation methods (e.g., [Lundberg and Lee, 2017]), it remains unclear in which settings the Banzhaf value may be preferable to the Shapley value. Our work provides the first theoretical characterization of the advantage of the Banzhaf value in terms of robustness. The empirical study by [Karczmarz et al., 2021] observes that the Banzhaf value is much more robust than Shapley value when the numerical precision is low in the computation, which validates our theoretical result.

We would like to note that Banzhaf value is a generalization of Banzhaf power index [Banzhaf III, 1964] which is designed for gauging the voting power of players in a simple voting game. In a simple voting game, the utility function $U : 2^N \rightarrow \{0, 1\}$ where $U(\emptyset) = 0$, $U(N) = 1$ and $U(S) \leq U(T)$ whenever $S \subseteq T$. In contrast, the setting of data valuation is more complicated and challenging as we do not assume any particular structure of the utility function $U$. There are also a lot of kinds of power indices are available, such as Shapley-Shubik index [Shapley, 1953], Holler index [Holler, 1982], and Deegan-Packel index [Deegan and Packel, 1978]. The interpretation and computation of these power indices are active topics in cooperative game theory (e.g., [Holler and Packel, 1983, Aziz, 2008]). In this work, we explore the most robust data value notion among the space of semivalues. Exploring the possibility of extending other kinds of cooperative solution concepts to data valuation is an interesting and promising future research direction.

**Efficient Estimation of Banzhaf and Shapley value.** Most of the estimation algorithms for Banzhaf and Shapley value are based on Monte Carlo techniques, especially when no prior knowledge is available about the structure of utility function $U$. The Simple Monte Carlo estimation for Shapley value (i.e., the Permutation Sampling) was mentioned in very early works [Mann and Shapley, 1960], and the sample complexity analysis of Permutation sampling for Shapley value can be found in [Maleki, 2015]. The sample complexity of Simple Monte Carlo method for Banzhaf value / Banzhaf power index [Merrill III, 1982] first appeared in [Bachrach et al., 2010]. Jia et al. [Jia et al., 2019b] improve the sample complexity of Monte Carlo-based Shapley estimation based on group testing technique. G-Shapley, TMC-Shapley [Ghorbani and Zou, 2019] and KNN-Shapley [Jia et al., 2019a] have been proposed as the efficient proxies of Shapley value. However, these are biased estimators for Shapley value in nature.

Another line of works study the estimation of Shapley and Banzhaf value in the problems with specific structures, e.g., (weighted) voting games [Owen, 1972, Fatima et al., 2008, Teneggi et al., 2021], and for the games where only few players have non-zero contribution [Jia et al., 2019b, Lin et al., 2022].
B Proofs and Additional Theoretical Results

B.1 Proofs for Theorems in the maintext

We omit the parameters of $U, N, \text{ or } w$ when it’s clear from the context.

**Theorem 5** (restated). For any $\tau > 0$, Banzhaf value $(w(k) = \frac{n^2}{2^{n-1}})$ achieves the largest safety margin $\text{Safe}(\tau; w) = \tau 2^{n/2-1}$ among all semivalues.

**Proof.** For any $\tau > 0$ and any pair of $(i, j)$, we denote

$$\text{Safe}_{i,j}(\tau; w) = \min_{U \in \mathcal{U}^{(\tau)}} \min_{\hat{U} \in \{\hat{U} : D_{i,j}(U; w)D_{i,j}(\hat{U}; w) \leq 0\}} \|\hat{U} - U\|$$

as the minimum amount of noise that is required to reverse the ranking of $(i, j)$ among all utility functions that $\tau$-distinguish $(i, j)$. Thus, the safety margin of the semivalue $w$ is

$$\text{Safe}(\tau; w) = \min_{i \neq j} \text{Safe}_{i,j}(\tau; w)$$

Note that $D_{i,j}(U; w)$ can be written as a dot product of $U$ and a column vector $a \in \mathbb{R}^{2^n}$

$$D_{i,j}(U; w) = a^T U$$

where each entry of $a$ corresponds to a subset $S \subseteq N$. We use $a[\cdot]$ to denote the value of $a$’s entry corresponds to $S$. For all $S \subseteq N \setminus \{i, j\}$, $a[S \cup i] = w(|S| + 1) + w(|S| + 2)$ and $a[S \cup j] = -(w(|S| + 1) + w(|S| + 2))$, and for all other subsets $a[S] = 0$. Let the perturbation $x = \hat{U} - U$ and matrix $A = aa^T$.

$$D_{i,j}(U; w)D_{i,j}(\hat{U}; w) = (a^T U)(a^T \hat{U})$$

$$= (a^T U)^T (a^T \hat{U})$$

$$= U^T aa^T \hat{U}$$

$$= U^T A \hat{U}$$

$$= U^T A(U + x)$$

Thus, if $D_{i,j}(U; w)D_{i,j}(\hat{U}; w) \leq 0$, the size of the perturbation $x$ must be at least

$$\|x\| \geq \frac{|U^T A U|}{\|U^T A\|}$$

$$= \frac{|U^T A U|}{\sqrt{U^T A A U}}$$

$$= \frac{|U^T A U|}{\sqrt{a^T a \sqrt{|U^T A U|}}}$$

$$= \sqrt{\frac{|U^T A U|}{a^T a}}$$
where (18) is because $AA = (aa^T)(aa^T) = a(a^T a)a^T = (a^T a)a^T = (a^T a)A$. This lower bound is achievable when we set $x$ on the direction of $U^T A$. Therefore, we have

$$\text{Safe}_{i,j}(\tau; w) = \min_{U \in U_{i,j}^{(\tau)}} \frac{|U^T A|}{a^T a}$$

(20)

To make the notations less cumbersome, denote $f(S) = w(|S| + 1) + w(|S| + 2)$, and $g(S) = U(S \cup i) - U(S \cup j)$. By expanding the expression, we have

$$\frac{|U^T A|}{a^T a} = \frac{\sum_{S \subseteq N \setminus \{i,j\}} \sum_{S_2 \subseteq N \setminus \{i,j\}} f(S_1) f(S_2) g(S_1) g(S_2)}{\sum_{S \subseteq N \setminus \{i,j\}} f^2(S)}$$

(21)

$$= \left( \sum_{S \subseteq N \setminus \{i,j\}} f(S_1) g(S_1) \right) \left( \sum_{S \subseteq N \setminus \{i,j\}} f(S_2) g(S_2) \right) \frac{1}{\sum_{S \subseteq N \setminus \{i,j\}} f^2(S)}$$

(22)

$$= \left( \sum_{S \subseteq N \setminus \{i,j\}} f(S) g(S) \right)^2 \frac{1}{\sum_{S \subseteq N \setminus \{i,j\}} f^2(S)}$$

(23)

$$= \frac{\sum_{k=1}^{n-1} \left( w(k) + w(k + 1) \right) \sum_{S \subseteq N \setminus \{i,j\}, |\tau| = k-1} \left( U(S \cup i) - U(S \cup j) \right)^2}{\sum_{k=1}^{n-1} \left( \binom{n-2}{k-1} \left( w(k) + w(k + 1) \right)^2 \right)}$$

(24)

Clearly, the minimum of (25) is achieved when

$$\binom{n-2}{k-1} \sum_{S \subseteq N \setminus \{i,j\}, |\tau| = k-1} \left( U(S \cup i) - U(S \cup j) \right) = \tau$$

(26)

for all $k$, i.e.,

$$\text{Safe}_{i,j}(\tau; w) = \tau \sqrt{\frac{\sum_{k=1}^{n-1} \left( \binom{n-2}{k-1} \left( w(k) + w(k + 1) \right) \right)^2}{\sum_{k=1}^{n-1} \left( \binom{n-2}{k-1} \left( w(k) + w(k + 1) \right)^2 \right)}}$$

(27)

Now, we want to find the optimal semivalue weight function $w$ that maximizes $\frac{\sum_{k=1}^{n-1} \left( \binom{n-2}{k-1} (w(k) + w(k + 1)) \right)^2}{\sum_{k=1}^{n-1} \left( \binom{n-2}{k-1} (w(k) + w(k + 1))^2 \right)}$.  

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Notice that
\[
\left( \sum_{k=1}^{n-1} \binom{n-2}{k-1} (w(k) + w(k+1)) \right)^2 \sum_{k=1}^{n-1} \binom{n-2}{k-1} (w(k) + w(k+1))^2
\]
\[
= \frac{\left( \sum_{k=1}^{n-1} \sqrt{\binom{n-2}{k-1}} \sqrt{\binom{n-2}{k-1}} (w(k) + w(k+1)) \right)^2}{\sum_{k=1}^{n-1} \binom{n-2}{k-1} (w(k) + w(k+1))^2}
\]
\[
\leq \frac{\sum_{k=1}^{n-1} \binom{n-2}{k-1} \sum_{k=1}^{n-1} \binom{n-2}{k-1} (w(k) + w(k+1))^2}{\sum_{k=1}^{n-1} \binom{n-2}{k-1} (w(k) + w(k+1))^2}
\]
\[
= \sum_{k=1}^{n-1} \binom{n-2}{k-1}
\]
\[
= 2^{n-2}
\]
where (30) is due to Cauchy-Schwarz inequality.

Note that this upper bound is achievable whenever \( w(|S| + 1) + w(|S| + 2) \) is a constant due to the equality condition of Cauchy-Schwarz, which the weight function of Banzhaf value clearly satisfies. Therefore, for any pair of data points \((i, j)\), Banzhaf value achieves the largest \( \text{Safe}_{i,j}(\tau; w) \), which means that Banzhaf value also achieves the largest safety margin \( \text{Safe}(\tau; w) \).

Further Discussion of Theorem 5. The safety margin in Theorem 5 characterizes the noise in utility that can be tolerated such that the ranking of exact semivalues calculated from clean utility match with that of exact semivalues calculated from noisy utility. However, calculating exact semivalues for a given utility function is NP-hard in general and in practice, one often resorts to evaluating the utility function at limited sampled subsets and then using these limited samples to approximate semivalues. Hence, a natural question to ask is whether we can characterize the maximally-tolerable utility noise on the limited sampled subsets such that the ranking of approximate semivalues calculated from the clean utility samples align with that of approximate semivalues calculated from the noisy samples. However, one issue with this type of characterization is that the “safety margin” in this case depends on both the expression of the semivalue (i.e., \( w \) that parametrizes the semivalue), as well as the underlying estimation algorithm for that semivalue. Since different semivalues have different estimation algorithms, such a result for different semivalues are not really comparable. On the other hand, our result in Theorem 5 lifts the dependence on the underlying estimation algorithm. As a consequence, it allows one to compare the robustness between different semivalues.

We also note that, Banzhaf value is not the unique semivalue that achieves the maximal robustness in the setup of Theorem 5. Any semivalues with a weight function \( w \) s.t. \( w(k) + w(k+1) \) is a constant also achieve the same safety margin. Such a semivalue must have \( w(1) = w(3) = w(5) = \ldots \) and \( w(2) = w(4) = w(6) = \ldots \). However, there’s no natural explanation for why the semivalue should weigh odd and even cardinalities differently. Hence, Banzhaf value is the only “reasonable” semivalue with maximal robustness.

Safety Margin of Leave-one-out error and Shapley value.

Corollary 10. For any \( \tau > 0 \), Leave-one-out error \( (w(k) = n1[k = n]) \) achieves safety margin \( \text{Safe}(\tau; w) = \tau \).
Proof. By plugging in $w(k) = n \mathbb{1}[k = n]$ to (27), we have $\text{Safe}_{i,j}(\tau; w) = \tau$ for any $i, j$, which leads to $\text{Safe}(\tau; w) = \tau$. \qed

Corollary 11. For any $\tau > 0$, Shapley value $(w(k) = \binom{n-1}{k-1}^{-1})$ achieves safety margin $\text{Safe}(\tau; w) \leq \tau(n - 1)$.

Proof. By plugging in $w(k) = \binom{n-1}{k-1}^{-1}$ to (27), we have

$$\text{Safe}_{i,j}(\tau; w) = \tau \frac{n - 1}{\sqrt{\sum_{k=1}^{n-1} \binom{n-2}{k-1}^{-1}}}$$

for any $i, j$, which leads to $\text{Safe}(\tau; w) = \tau(n - 1)$. \qed

Remark. Note that the safety margin of the Shapley value in (33) is greater than $\tau$, which means that Shapley value’s safety margin is greater than that of the LOO error. Our results shed light on a common observation in the past works [Ghorbani and Zou, 2019, Jia et al., 2019c] that the Shapley value often outperforms the LOO error in identifying low-quality training data.

Theorem 6 (restated). $\hat{\phi}_{MC}$ is an $(\varepsilon, \delta)$-approximation to the exact Banzhaf value in $\ell_2$-norm with $O(\frac{n^2}{\varepsilon^2} \log(\frac{n}{\delta}))$ calls of $U(\cdot)$, and in $\ell_\infty$-norm with $O(\frac{n}{\varepsilon} \log(\frac{n}{\delta}))$ calls of $U(\cdot)$.

Proof. Let $S = \{S_1, \ldots, S_m\}$ be the samples used for computing $\hat{\phi}_{MC}(i)$. Since the marginal contribution $U(S \cup i) - U(S)$ is always bounded between $[-1, 1]$, by Hoeffding, we have

$$\Pr \left[ \left| \hat{\phi}_{MC}(i) - \phi(i) \right| \geq \varepsilon \right] \leq 2 \exp \left( -2m\varepsilon^2 \right)$$

which holds for every $i \in N$.

Thus, with union bound, for $\ell_2$-norm we have

$$\Pr_{\hat{\phi}_{MC}} \left[ \left\| \hat{\phi}_{MC} - \phi \right\|_2 \geq \varepsilon \right] = 1 - \Pr_{\hat{\phi}_{MC}} \left[ \left\| \hat{\phi}_{MC} - \phi \right\|_2 \leq \varepsilon^2 \right] \leq 1 - \Pr_{\hat{\phi}_{MC}} \left[ \bigcap_{i} \left| \hat{\phi}_{MC}(i) - \phi(i) \right| \leq \varepsilon / \sqrt{n} \right] \leq \Pr_{\hat{\phi}_{MC}} \left[ \bigcup_{i} \left| \hat{\phi}_{MC}(i) - \phi(i) \right| \geq \varepsilon / \sqrt{n} \right] \leq \sum_{i=1}^{n} \Pr_{\hat{\phi}_{MC}} \left[ \left| \hat{\phi}_{MC}(i) - \phi(i) \right| \geq \varepsilon / \sqrt{n} \right] \leq 2n \exp \left( -2m\varepsilon^2 / n \right)$$

By setting $2n \exp \left( -2m\varepsilon^2 / n \right) \leq \delta$, we get $m \geq \frac{n}{2\varepsilon^2} \log \left( \frac{2n}{\delta} \right) = O \left( \frac{n}{\varepsilon^2} \log(\frac{n}{\delta}) \right)$. However, this $m$ only corresponds to the number of samples used to estimate a single $\phi(i)$, so the total number of samples required is $O \left( \frac{n^2}{\varepsilon^2} \log(\frac{n}{\delta}) \right)$.
For $\ell_\infty$-norm we have
\[
\Pr_{\hat{\phi}_{MC}} \left[ \|\hat{\phi}_{MC} - \phi\|_\infty \geq \varepsilon \right] = \Pr_{\hat{\phi}_{MC}} \left[ \bigcup_i \left| \hat{\phi}_{MC}(i) - \phi(i) \right| \geq \varepsilon \right] = \sum_{i=1}^{n} \Pr_{\hat{\phi}_{MC}} \left[ \left| \hat{\phi}_{MC}(i) - \phi(i) \right| \geq \varepsilon \right] \leq 2n \exp(-2m\varepsilon^2) \tag{40}
\]

By setting $2n \exp(-2m\varepsilon^2) \leq \delta$, we get $m \geq \frac{1}{2\varepsilon^2} \log \left( \frac{2n}{\delta} \right) = O \left( \frac{1}{\varepsilon^2} \log \left( \frac{n}{\delta} \right) \right)$. However, this $m$ only corresponds to the number of samples used to estimate a single $\phi(i)$, so the total number of samples required is $O \left( \frac{1}{\varepsilon^2} \log \left( \frac{n}{\delta} \right) \right)$.

**Theorem 7** (restated). $\hat{\phi}_{MSR}$ is an $(\varepsilon, \delta)$-approximation to the exact Banzhaf value in $\ell_2$-norm with $O \left( \frac{1}{\varepsilon^2} \log \left( \frac{n}{\delta} \right) \right)$ calls of $U(\cdot)$, and in $\ell_\infty$-norm with $O \left( \frac{1}{\varepsilon^2} \log \left( \frac{n}{\delta} \right) \right)$ calls of $U(\cdot)$.

**Proof.** Since $S = \{S_1, \ldots, S_m\}$ each i.i.d. drawn from Unif($2^N$), it is easy to see that the size of sampled subsets that include data point $i$ follows binomial distribution $|S_\ni| \sim \text{Bin}(m, 0.5)$, and $|S_\ni| = m - |S_{\ni}|$.

We first define an alternative estimator
\[
\tilde{\phi}(i) = \frac{1}{m/2} \sum_{S \in S_{\ni}} U(S) - \frac{1}{m/2} \sum_{S \in S_{\ni}} U(S) \tag{43}
\]
which is independent of $|S_{\ni}|$ and $|S_{\ni}|$. When both $|S_{\ni}|$ and $|S_{\ni}| > 0$, we have
\[
\left| \hat{\phi}(i) - \tilde{\phi}(i) \right| = \left| \left( \frac{1}{|S_{\ni}|} - \frac{1}{m/2} \right) \sum_{S \in S_{\ni}} U(S) - \left( \frac{1}{|S_{\ni}|} - \frac{1}{m/2} \right) \sum_{S \in S_{\ni}} U(S) \right| \tag{44}
\]
\[
\leq 1 - \frac{2|S_{\ni}|}{m} + 1 - \frac{2|S_{\ni}|}{m} \tag{45}
\]
\[
= 2 \left| 1 - \frac{2|S_{\ni}|}{m} \right| \tag{46}
\]
\[
= \frac{4}{m} \left| |S_{\ni}| - \frac{m}{2} \right| \tag{47}
\]
where (46) is due to $U(S) \leq 1$ and (47) is due to $|S_{\ni}| = m - |S_{\ni}|$. When one of $|S_{\ni}|$ and $|S_{\ni}| = 0$, this upper bound also clearly holds.

Since $|S_{\ni}| \sim \text{Bin}(m, 0.5)$, by Hoeffding inequality we have
\[
\Pr \left[ \left| |S_{\ni}| - \frac{m}{2} \right| \geq \Delta \right] \leq 2 \exp \left( -\frac{2\Delta^2}{m} \right) \tag{49}
\]

Hence, with probability at least $1 - 2 \exp \left( -\frac{2\Delta^2}{m} \right)$, we have
\[
\left| \hat{\phi}(i) - \tilde{\phi}(i) \right| \leq \frac{4\Delta}{m} \tag{50}
\]
Since
\[
\tilde{\phi}(i) = \frac{2}{m} \left( \sum_{S \in \mathcal{S}_i} U(S) - \sum_{S \in \mathcal{S}_{\bar{i}}} U(S) \right)
\]
(51)

\[
= \frac{1}{m} \sum_{S \in \mathcal{S}} 2U(S)\text{sign}(i, S)
\]
(52)

where \( \text{sign}(i, S) = 21[i \in S] - 1 \in \{\pm 1\} \). Thus, \( 2U(S)\text{sign}(i, S) \in [-2, 2] \) and we can apply Hoeffding to bound the tail of \( |\tilde{\phi}(i) - \phi(i)| \):
\[
\Pr \left[ |\tilde{\phi}(i) - \phi(i)| \geq t \right] \leq 2 \exp \left( -\frac{mt^2}{8} \right)
\]
(53)

Now we bound \( |\tilde{\phi}(i) - \phi(i)| \) as follows:
\[
\Pr \left[ |\tilde{\phi}(i) - \phi(i)| \geq \epsilon \right] = \Pr \left[ |\tilde{\phi}(i) - \phi(i)| \geq \epsilon \left| |\mathcal{S}_{\bar{i}}| - \frac{m}{2} \right| \leq \Delta \right] \Pr \left[ |\mathcal{S}_{\bar{i}}| - \frac{m}{2} \leq \Delta \right] + \Pr \left[ |\mathcal{S}_{\bar{i}}| - \frac{m}{2} > \Delta \right] \Pr \left[ |\mathcal{S}_{\bar{i}}| - \frac{m}{2} > \Delta \right]
\]
(54)

\[
\leq \Pr \left[ |\tilde{\phi}(i) - \phi(i)| \geq \epsilon \left| |\mathcal{S}_{\bar{i}}| - \frac{m}{2} \right| \leq \Delta \right] + 2 \exp \left( -\frac{2\Delta^2}{m} \right)
\]
(55)

\[
\leq \Pr \left[ |\phi(i) - \phi(i)| \geq \epsilon \left| |\mathcal{S}_{\bar{i}}| - \frac{m}{2} \right| \leq \Delta \right] + 2 \exp \left( -\frac{2\Delta^2}{m} \right)
\]
(56)

\[
\leq \Pr \left[ |\phi(i) - \phi(i)| \geq \epsilon \left| |\mathcal{S}_{\bar{i}}| - \frac{m}{2} \right| \leq \Delta \right] + 2 \exp \left( -\frac{2\Delta^2}{m} \right)
\]
(57)

\[
\leq \frac{1 - 2 \exp \left( -\frac{2\Delta^2}{m} \right)}{1 - 2 \exp \left( -\frac{2\Delta^2}{m} \right)} + 2 \exp \left( -\frac{2\Delta^2}{m} \right)
\]
(58)

\[
\leq \frac{2 \exp \left( -\frac{1}{8}m(\epsilon - \frac{4\Delta}{m})^2 \right) + 2 \exp \left( -\frac{2\Delta^2}{m} \right)}{1 - 2 \exp \left( -\frac{2\Delta^2}{m} \right)}
\]
(59)

\[
\leq 3 \exp \left( -\frac{1}{8}m \left( \epsilon - \frac{4\Delta}{m} \right)^2 \right) + 2 \exp \left( -\frac{2\Delta^2}{m} \right)
\]
(60)

where the last inequality holds whenever \( 1 - 2 \exp \left( -\frac{2\Delta^2}{m} \right) \geq \frac{2}{3} \).

We can then optimize this bound by setting \( -\frac{1}{8}m \left( \epsilon - \frac{4\Delta}{m} \right)^2 = -\frac{2\Delta^2}{m} \), where we obtain \( \Delta = \frac{m\epsilon}{8} \), and the bound becomes
\[
\Pr \left[ |\tilde{\phi}(i) - \phi(i)| \geq \epsilon \right] \leq 3 \exp \left( -\frac{1}{8}m \left( \epsilon - \frac{4\Delta}{m} \right)^2 \right) + 2 \exp \left( -\frac{2\Delta^2}{m} \right)
\]
(61)

\[
= 5 \exp \left( -\frac{m\epsilon^2}{32} \right)
\]
(62)

By union bound, we have
\[
\Pr_{\tilde{\phi}_{\text{MSR}}} \left[ \left\| \tilde{\phi}_{\text{MSR}} - \phi \right\|_2 \geq \epsilon \right] \leq 5n \exp \left( -\frac{m\epsilon^2}{32n} \right)
\]
(63)

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and

\[ \Pr_{\hat{\phi}_{\text{MSR}}} \left[ \left\| \hat{\phi}_{\text{MSR}} - \phi \right\|_\infty \geq \varepsilon \right] \leq 5n \exp \left( -\frac{m\varepsilon^2}{32} \right) \]  

(65)

By setting \( \delta \leq 5n \exp \left( -\frac{m\varepsilon^2}{32n} \right) \), we obtain the sample complexity \( O \left( \frac{n}{\varepsilon^2 \log \left( \frac{n}{\delta} \right)} \right) \) for \( \ell_2 \) norm, and by setting \( \delta \leq 5n \exp \left( -\frac{m\varepsilon^2}{32} \right) \), we obtain the sample complexity \( O \left( \frac{1}{\varepsilon^2 \log \left( \frac{n}{\delta} \right)} \right) \) for \( \ell_\infty \)-norm.

\[ \square \]

### B.2 MSR Estimator does not Extend to Shapley Value and Other Known Semi-values

In this section, we provide proofs and more discussion about why the existence of MSR estimator is a unique advantage of Banzhaf value.

**Numerical Instability.** It is easy to see that semivalue can be written as the expectation of weighted marginal contribution

\[ \phi_{\text{semi}}(i; U, N, w) := \frac{1}{n} \sum_{k=1}^{n} w(k) \sum_{S \subseteq N \setminus \{i\}, |S| = k-1} [U(S \cup i) - U(S)] \]  

(66)

\[ = \mathbb{E}_{S \sim \text{Unif}(2^N \setminus i)} \left[ \frac{2^{n-1}w(|S| + 1)}{n} U(S \cup i) - U(S) \right] \]  

(67)

\[ = \mathbb{E}_{S \sim \text{Unif}(2^N \setminus i)} \left[ \frac{2^{n-1}w(|S| + 1)}{n} U(S \cup i) \right] - \mathbb{E}_{S \sim \text{Unif}(2^N \setminus i)} \left[ \frac{2^{n-1}w(|S| + 1)}{n} U(S) \right] \]  

(68)

\[ = \mathbb{E}_{S \sim \text{Unif}(\{S \in 2^N : S \ni i\}) \left[ \frac{2^{n-1}w(|S|)}{n} U(S) \right] - \mathbb{E}_{S \sim \text{Unif}(2^N \setminus i)} \left[ \frac{2^{n-1}w(|S| + 1)}{n} U(S) \right] \]  

(69)

Hence, a straightforward way to design MSR estimator for arbitrary semivalue is to sample \( S = \{S_1, \ldots, S_m\} \) each i.i.d. drawn from \( \text{Unif}(2^N) \), and estimate \( \phi(i) \) as

\[ \hat{\phi}_{\text{MSR}}(i) = \frac{1}{|S_i|} \sum_{S \in S_i \setminus S_{\bar{i}}} \frac{2^{n-1}w(|S|)}{n} U(S) - \frac{1}{|S_{\bar{i}}|} \sum_{S \in S_{\bar{i}}} \frac{2^{n-1}w(|S| + 1)}{n} U(S) \]  

(70)

For Shapley value, \( w(|S|) = (\frac{n-1}{|S|-1})^{-1} \), which makes the MSR estimator for Shapley value becomes

\[ \hat{\phi}_{\text{MSR}}(i) = \frac{1}{|S_i|} \sum_{S \in S_i \setminus S_{\bar{i}}} \frac{1}{n} \left( \frac{n-1}{|S|-1} \right)^{-1} U(S) - \frac{1}{|S_{\bar{i}}|} \sum_{S \in S_{\bar{i}}} \frac{1}{n} \left( \frac{n-1}{|S|} \right)^{-1} U(S) \]  

(71)

which is numerically unstable for large \( n \) due to the combinatorial coefficients.

**Impossible to construct a special sampling distribution for MSR.** The MSR estimator for Banzhaf value samples from \( \text{Unif}(2^N) \) since for a random set \( S \sim \text{Unif}(2^N) \), we have its conditional distribution \( S|S \ni i \sim \text{Unif}(2^{N \setminus i}) \) and \( S|S \ni i \sim \text{Unif}(\{S \in 2^N : S \ni i\}) \), which exactly matches the two distributions the expectation in (70) is taken over for Banzhaf value.
For a semivalue with weight function $w$, can we design a similar distribution $D$ over $2^N$ so that $\phi_{\text{semi}}(i; U, N, w) = \mathbb{E}_{S \sim D \mid D \ni i}[U(S)] - \mathbb{E}_{S \sim D \mid D \notin i}[U(S)]$? The answer is unfortunately negative. Note that in order to write $\phi_{\text{semi}}(i; U, N, w)$ in this way, we must have

$$\Pr[D = S | i \in S] = \frac{1}{n} w(|S| + 1)$$ (73)

$$\Pr[D = S | i \notin S] = \frac{1}{n} w(|S|)$$ (74)

for any $i \in N$. Now, we consider a particular $S$ s.t. $i \notin S, j \in S$. Denote $x = \Pr[i \notin D]$, $y = \Pr[j \notin D]$, and $k = |S| + 1$. By Bayes theorem, we have

$$\Pr[D = S | i \notin S, j \in S] = \frac{\Pr[j \in D | D = S, i \notin D] \Pr[D = S | i \notin D]}{\Pr[j \in D]}$$ (75)

$$= \frac{w(k - 1)}{n(1 - y)}$$ (76)

$$= \Pr[i \notin D | D = S, j \in D] \frac{\Pr[D = S | j \in D]}{\Pr[i \notin D]}$$ (77)

$$= \frac{w(k)}{nx}$$ (78)

Thus we have $w(k - 1)x = w(k)(1 - y)$. Similarly, consider a $S'$ of the same size s.t. $i \in S, j \notin S$, we obtain $w(k - 1)y = w(k)(1 - x)$.

Given

$$w(k - 1)x = w(k)(1 - y)$$ (80)

$$w(k - 1)y = w(k)(1 - x)$$ (81)

If $x = y$, then we have $x = \frac{w(k - 1)}{w(k - 1) + w(k)}$ which clearly depends on $k$ unless $w(1), w(2), \ldots, w(n)$ is a geometric series ($w(k - 1) + w(k)$ cannot be 0 for all $k$, and $x$ can also not be 0). The only known semivalue-based data valuation method that satisfy this property is Banzhaf value.

If $x \neq y$, then we have $w(k - 1)(x - y) = w(k)(x - y)$, which clearly leads to $w(k - 1) = w(k)$ where Banzhaf value is still the only choice.

### B.3 Improved Group Testing-based Estimator for Shapley Value

[Jia et al., 2019b] propose an estimation algorithm for Shapley value that achieves $\widetilde{O}(n)$ sample complexity. The estimation algorithm is inspired by the group testing theory [Zhou et al., 2014]. Instead of directly estimating the Shapley value of each data point $\phi_{\text{shap}}(i)$, the key idea of Group Testing-based estimation algorithm is to estimate the difference of the Shapley value between every pair of data points $\phi_{\text{shap}}(i) - \phi_{\text{shap}}(j)$.

**Lemma 12.** For any $i, j \in N$, the difference in Shapley value between $i$ and $j$ is

$$\Delta_{\text{shap}}^{(i,j)} := \phi_{\text{shap}}(i) - \phi_{\text{shap}}(j) = \frac{1}{n - 1} \sum_{S \subseteq N \setminus \{i, j\}} \left( \frac{1}{|S|} \right)^{n - 2} [U(S \cup i) - U(S \cup j)]$$ (82)
The algorithm of Group Testing designs a distribution over the cardinalities of data subset \( q(k) = \frac{1}{Z} \left( \frac{1}{k} + \frac{1}{n-k} \right) \) for \( k = 1, \ldots, n-1 \), where \( Z = 2\sum_{k=1}^{n-1} \frac{1}{k} \) is the normalization factor. The original Group Testing algorithm with sampling budget \( m \) proceeds as follows:

1. Initialize a matrix \( A \in \mathbb{R}^{m \times n} \), \( b \in \mathbb{R}^m \).

2. For \( t = 1, \ldots, m \), repeat the following sampling procedure: draw \( k_t \sim q \); sample a subset \( S_t \) of size \( k_t \) from \( N \) uniformly at random; set \( A_{t,i} \leftarrow 1 \) for all \( i \in S_t \), and \( A_{t,i} \leftarrow 0 \) for all \( i \notin S_t \); set \( b_t \leftarrow U(S_t) \).

3. \( \hat{\Delta}_{\text{shap}}^{(i,j)} = \frac{Z}{m} \sum_{t=1}^{m} b_t (A_{t,i} - A_{t,j}) \) for \( i = 1, \ldots, n \) and \( j = 1, \ldots, n \).

4. Compute \( \hat{\phi}_{\text{shap}} \) by solving the feasibility problem \( \sum_{i=1}^{n} \hat{\phi}_{\text{shap}}(i) = U(N) \) \( \varepsilon/2\sqrt{n} \) for every pair of \( i, j \) in \( \{1, \ldots, n\} \).

To see the correctness of the above algorithm, we cite the following results from [Jia et al., 2019b].

**Lemma 13** ([Jia et al., 2019b]). \( \mathbb{E} \left[ \hat{\Delta}_{\text{shap}}^{(i,j)} \right] = \Delta_{\text{shap}}^{(i,j)} \).

**Lemma 14** ([Jia et al., 2019b]). Suppose that \( \hat{\Delta}_{\text{shap}}^{(i,j)} \) is an \( (\varepsilon/(2\sqrt{n}), \delta/(n(n-1))) \)-approximation to \( \phi_{\text{shap}}(i) - \phi_{\text{shap}}(j) \). Then, the solution to the feasibility problem

\[
\sum_{i=1}^{n} \hat{\phi}_{\text{shap}}(i) = U(N) \\
\left| (\hat{\phi}_{\text{shap}}(i) - \hat{\phi}_{\text{shap}}(j)) - \hat{\Delta}_{\text{shap}}^{(i,j)} \right| \leq \frac{\varepsilon}{2\sqrt{n}} \quad \forall i, j \in \{1, \ldots, n\}
\]

is an \( (\varepsilon, \delta) \)-approximation in \( \ell_2 \)-norm.

By Lemma 14, we know that the sample size \( m \) should be enough such that \( \hat{\Delta}_{\text{shap}}^{(i,j)} \) is an \( (\varepsilon/(2\sqrt{n}), \delta/(n(n-1))) \)-approximation to \( \phi_{\text{shap}}(i) - \phi_{\text{shap}}(j) \) for every pair of \( i, j \in N \).

**Theorem 15** ([Jia et al., 2019b]). The original Group Testing-based estimation achieves \( (\varepsilon, \delta) \)-approximation in \( \ell_2 \) norm with \( O \left( \frac{n^2}{\varepsilon} (\log n)(\log \frac{n^2}{\delta}) \right) \) samples.

We refer the readers to the original paper [Jia et al., 2019b] for detailed proof. However, we want to mention that the term \( \log \frac{n^2}{\delta} \) is due to the fact that the algorithm requires the estimate of \( \hat{\Delta}_{\text{shap}}^{(i,j)} \) to be within \( \frac{\varepsilon}{2\sqrt{n}} \) error for every pair of \( i, j \) with probability at least \( 1 - \delta \), which results in requiring \( \frac{\varepsilon}{\sqrt{n}} \) error with probability at least \( 1 - \frac{\delta}{n(n-1)} \) confidence for each pair of \( i, j \). While the above algorithm achieves \( O(n) \) sample complexity asymptotically, it can still be sample-inefficient in practice [Jia et al., 2019b, Wang et al., 2020].

Do we really need to estimate the Shapley value differences for every pair of data points? If we already know the Shapley value of a particular player \( * \), we can just estimate \( \phi_{\text{shap}}(i) - \phi_{\text{shap}}(*) \) for every \( i \in N \), and compute \( \hat{\phi}_{\text{shap}}(i) = \phi_{\text{shap}}(*) + \hat{\Delta}_{\text{shap}}^{(i,*)} \). Here, we introduce a simple but elegant trick called **Dummy Player**.

**Dummy Player Trick.** Note that the dummy player axiom of Shapley value says that for a player \( i \), if \( U(S \cup i) = U(S) \) for all \( S \subseteq N \setminus i \), then \( \phi_{\text{shap}}(i) = 0 \). Given a training dataset \( N = \{1, \ldots, n\} \),
we augment it by adding a dummy player called \(n+1\), i.e., \(N' = N \cup \{n+1\}\). For any utility function \(U\), we augment it by setting \(U'(S) = U(S)\) and \(U'(S \cup n + 1) = U(S)\) for all \(S \subseteq N\). Thus, we have \(\phi_{\text{shap}}(n+1; U') = 0\). We can modify the Group Testing-based algorithm as follows: The algorithm of Group Testing designs a distribution over the cardinalities of data subset \(q(k) = \frac{1}{Z} \left( \frac{1}{k} + \frac{1}{n+1-k} \right)\) for \(k = 1, \ldots, n\), where \(Z = 2 \sum_{i=1}^{n} \frac{1}{k}\) is the normalization factor. The modified Group Testing algorithm with sampling budget \(m\) proceeds as follows:

1. Initialize a matrix \(A \in \mathbb{R}^{m \times (n+1)}\), \(b \in \mathbb{R}^m\).
2. For \(t = 1, \ldots, m\), repeat the following sampling procedure: draw \(k_t \sim q\); sample a subset \(S_t\) of size \(k_t\) from \(N\) uniformly at random; set \(A_{t,i} \leftarrow 1\) for all \(i \in S_t\), and \(A_{t,i} \leftarrow 0\) for all \(i \notin S_t\); set \(b_t \leftarrow U'(S_t)\).
3. \(\Delta_{\text{shap}}^{(i,n+1)} = \frac{Z}{m} \sum_{t=1}^{m} b_t (A_{t,i} - A_{t,n+1})\) for \(i = 1, \ldots, n\).
4. \(\phi_{\text{shap}}(i) = \Delta_{\text{shap}}^{(i,n+1)}\) for \(i = 1, \ldots, n\).

We show that the augmentation from \(U\) to \(U'\) does not change the Shapley value of any data points \(i \in N\).

**Theorem 16.** \(\phi_{\text{shap}}(i; U') = \phi_{\text{shap}}(i; U)\) for all \(i \in N\).

**Proof.**

\[
\phi_{\text{shap}}(i; U') = \frac{1}{n + 1} \sum_{k=0}^{n} \binom{n}{k}^{-1} \sum_{S \subseteq N \setminus \{i\} \setminus S \subseteq k} U'(S \cup i) - U'(S) 
\]

\[
= \frac{1}{n + 1} \sum_{k=0}^{n-1} \sum_{S \subseteq N \setminus \{i\} \setminus S \subseteq k} \left[ \binom{n}{k}^{-1} U'(S \cup i) - U'(S) \right] + \binom{n}{k+1}^{-1} \left[ U'(S \cup \{i, n+1\}) - U'(S \cup n + 1) \right] 
\]

\[
= \frac{1}{n + 1} \sum_{k=0}^{n-1} \sum_{S \subseteq N \setminus \{i\} \setminus S \subseteq k} \left[ \binom{n}{k}^{-1} + \binom{n}{k+1}^{-1} \right] \left[ U'(S \cup i) - U(S) \right] 
\]

\[
= \frac{1}{n + 1} \sum_{k=0}^{n-1} \sum_{S \subseteq N \setminus \{i\} \setminus S \subseteq k} \frac{n+1}{n} \binom{n-1}{k}^{-1} \left[ U'(S \cup i) - U(S) \right] 
\]

\[
= \frac{1}{n} \sum_{k=0}^{n-1} \sum_{S \subseteq N \setminus \{i\} \setminus S \subseteq k} \binom{n-1}{k}^{-1} \left[ U'(S \cup i) - U(S) \right] 
\]

\[
= \phi_{\text{shap}}(i; U) 
\]

**Theorem 17 ([Jia et al., 2019b]).** The modified Group Testing-based estimation achieves \((\varepsilon, \delta)\)-approximation in \(\ell_2\) norm with \(O\left(\frac{n+1}{\varepsilon^2} (\log(n+1))(\log \frac{n}{\delta})\right)\) samples.
Yao’s minimax principle calls, and approximation in
Proof sketch: To achieve $(\varepsilon, \delta)$-approximation in $\ell_2$-norm, one need $(\varepsilon/\sqrt{n}, \delta/n)$-approximation to
$\phi_{\text{shap}}(i) = \Delta_{\text{shap}}^{(i,n+1)}$ for each $i = 1, \ldots, n$.

While the sample complexity of the modified group testing estimator is still $O(n)$ asymptotically, it improves the sample complexity of the original group testing estimator by a factor of 2 since we only need to estimate $n$ pairs of Shapley differences instead of $n^2$ pairs.

### B.4 Lower Bound for Banzhaf Value Estimator

**Theorem 8.** Every (possibly randomized) Banzhaf value estimation algorithm that achieves $(\varepsilon, \delta)$-approximation in $\ell_\infty$-norm for constant $\delta \in (0, 1/2)$ has sample complexity at least $\Omega(1/\varepsilon^2)$.

**Proof.** To show the lower bound of the sample complexity for Banzhaf value estimation, we use Yao’s minimax principle: to show a lower bound on a randomized algorithm, it suffices to define a distribution on some family of instances and show a lower bound for deterministic algorithms on this distribution.

Fix $\varepsilon \in (0, 1)$. We define the collection of instance $\mathcal{I}_0$ as all utility functions $U$ such that $U(S) = U(S \cup n)$ for all $S \subseteq [n-1]$. We define the collection of instance $\mathcal{I}_1$ as all utility functions $U$ s.t. there are exactly $2^n - 1(2\varepsilon)$ of the $S \subseteq [n-1]$ has $U(S) = 0, U(S \cup n) = 1$, and for all other $S$ we have $U(S) = U(S \cup n)$. We define a distribution over $\mathcal{I}_0 \cup \mathcal{I}_1$ by first randomly pick $\mathcal{I}_0$ or $\mathcal{I}_1$ with probability $1/2$, and then pick a utility function from the selected instance class uniformly at random.

For any $U \in \mathcal{I}_0$, we have $\phi(n; U) = 0$, and for any $U \in \mathcal{I}_1$, we have $\phi(n; U) = 2^{n-1}(2\varepsilon) = 2\varepsilon$. Thus, in order to achieve $\|\hat{\phi} - \phi\|_\infty < \varepsilon$, the estimator must be able to distinguish between whether the utility function is from $\mathcal{I}_0$ or $\mathcal{I}_1$. For this, it needs to identify at least one $S \subseteq [n-1]$ s.t. $U(S) = 0, U(S \cup n) = 1$. However, since those $S$ are chosen uniformly at random, no matter what sampling strategy the algorithm has, each query succeeds with probability at most $2^{n-1}(2\varepsilon)/2^n = 2\varepsilon$. Thus, for $m$ queries, the total failure probability is at least $(1 - 2m\varepsilon)/2$. To make the failure probability at most $\delta$, we need number of samples $m$ s.t. $(1 - 2m\varepsilon)/2 \leq \delta$, which leads to the lower bound $m \geq \frac{1 - 2\delta}{2\varepsilon}$. Thus, we have $m \in \Omega(\frac{1}{\varepsilon})$.

### B.5 Robustness of MSR Estimator

Recall that

$$\tilde{\phi}_{\text{MSR}}(i) = \frac{1}{|S_{\tilde{g}_i}|} \sum_{S \in S_{\tilde{g}_i}} \tilde{U}(S) - \frac{1}{|S_{\tilde{g}'_i}|} \sum_{S \in S_{\tilde{g}'_i}} \tilde{U}(S)$$

(90)

**Theorem 9.** When $\|U - \tilde{U}\|_2 \leq \gamma$, $\tilde{\phi}_{\text{MSR}}$ is $(\varepsilon + \frac{\gamma \sqrt{n}}{2n/2^{n/2}}, \delta)$-approximation in $\ell_2$-norm with $O(\frac{n}{\varepsilon^2} \log(\frac{n}{\delta}))$ calls, and $(\varepsilon + \frac{\gamma}{2n/2^{n/2}}, \delta)$-approximation in $\ell_\infty$-norm with $O(\frac{1}{\varepsilon} \log(\frac{n}{\delta}))$ calls to $\tilde{U}$.

**Proof.** Note that for each $i \in N$,

$$|\tilde{\phi}(i) - \phi(i)| \leq |\tilde{\phi}(i) - \hat{\phi}(i)| + |\hat{\phi}(i) - \phi(i)|$$

(91)
From Theorem 7, we have

\[
\Pr_{\hat{\phi}} \left[ \left| \hat{\phi}(i) - \phi(i) \right| \geq \Delta \right] \leq 5 \exp \left( -\frac{m}{32} \Delta^2 \right) \tag{92}
\]

Now we bound \( \left| \tilde{\phi}(i) - \hat{\phi}(i) \right| \).

\[
\left| \tilde{\phi}(i) - \hat{\phi}(i) \right| = \left| \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} (U(S) - \hat{U}(S)) - \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} (U(S) - \hat{U}(S)) \right| \tag{93}
\]

\leq \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} \left| U(S) - \hat{U}(S) \right| + \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} \left| U(S) - \hat{U}(S) \right| \tag{94}

Given \( \| U - \hat{U} \| \leq \gamma \), we bound \( \left| \tilde{\phi}(i) - \hat{\phi}(i) \right| \) as follows:

\[
\Pr \left[ \left| \tilde{\phi}(i) - \hat{\phi}(i) \right| \geq \varepsilon \right] \leq \Pr \left[ \left| \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} \left| U(S) - \hat{U}(S) \right| + \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} \left| U(S) - \hat{U}(S) \right| \geq \varepsilon \right] \tag{95}
\]

\leq \Pr \left[ \left| \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} \left| U(S) - \hat{U}(S) \right| + \frac{1}{|S_{\exists_i}|} \sum_{S \in S_{\exists_i}} \left| U(S) - \hat{U}(S) \right| \geq \varepsilon \left| |S_{\exists_i}| - \frac{m}{2} \right| \leq \Delta \right] \tag{96}

+ 2 \exp \left( -\frac{2 \Delta^2}{m} \right) \tag{97}

\leq \frac{\Pr \left[ \frac{2}{m} \sum_{S \subseteq S} \left| U(S) - \hat{U}(S) \right| \geq \varepsilon - \frac{4 \Delta}{m} \right]}{1 - 2 \exp \left( -\frac{2 \Delta^2}{m} \right)} + 2 \exp \left( -\frac{2 \Delta^2}{m} \right) \tag{98}

By \( \| U - \hat{U} \| \leq \gamma \), we have

\[
\mathbb{E}[|U(S) - \hat{U}(S)|] = \frac{1}{2^m} \sum_{S \subseteq N} |U(S) - \hat{U}(S)| = \frac{1}{2^m} \| U - \hat{U} \|_1 \leq \frac{\sqrt{2^m}}{2^n} \| U - \hat{U} \| = \frac{\gamma}{2^{n/2}} \tag{100}
\]
Set $\varepsilon' = \varepsilon - \frac{\gamma}{2^{n/2-1}}$. Thus

$$ (99) \quad \Pr \left[ \frac{2}{m} \sum_{S \subseteq S} \left| U(S) - \tilde{U}(S) \right| - \frac{\gamma}{2^{n/2-1}} \geq \varepsilon' - \frac{4\Delta}{m} \right] \leq \frac{1}{1 - 2 \exp \left( - \frac{2\Delta^2}{m} \right)} + 2 \exp \left( - \frac{2\Delta^2}{m} \right) $$

Therefore,

$$ (100) \quad \Pr \left[ \frac{2}{m} \sum_{S \subseteq S} \left| U(S) - \tilde{U}(S) \right| - \frac{\gamma}{2^{n/2-1}} \geq \varepsilon' - \frac{4\Delta}{m} \right] \leq \frac{1}{1 - 2 \exp \left( - \frac{2\Delta^2}{m} \right)} + 2 \exp \left( - \frac{2\Delta^2}{m} \right) $$

By union bound, we have

$$ (101) \quad \Pr \left[ \left\| \phi(i) - \tilde{\phi}(i) \right\| \geq \varepsilon + \frac{\gamma}{2^{n/2-1}} \right] \leq 5 \exp \left( - \frac{m}{32} \varepsilon^2 \right) $$

Therefore,

$$ (102) \quad \Pr \left[ \left\| \phi(i) - \tilde{\phi}(i) \right\| \geq \varepsilon + \frac{\gamma}{2^{n/2-1}} \right] \leq \Pr \left[ \left\| \phi(i) - \tilde{\phi}(i) \right\| + \left\| \tilde{\phi}(i) - \phi(i) \right\| \geq \varepsilon + \frac{\gamma}{2^{n/2-1}} \right] $$

By setting $\delta \leq 10n \exp \left( - \frac{m\varepsilon^2}{128} \right)$, we obtain the sample complexity $O \left( \frac{n}{\varepsilon} \log \left( \frac{n}{\delta} \right) \right)$ for $\ell_2$-norm, and by setting $\delta \leq 10n \exp \left( - \frac{m\varepsilon^2}{128} \right)$, we obtain the sample complexity $O \left( \frac{1}{\varepsilon^2} \log \left( \frac{n}{\delta} \right) \right)$ for $\ell_\infty$-norm. 

32
B.6 Stability of Banzhaf value in $\ell_2$-norm

As mentioned previously, we can alternatively view a semivalue as a function $\phi : \mathbb{R}^{2^n} \to \mathbb{R}^n$ which takes a utility function $U \in \mathbb{R}^{2^n}$ as input, and output the values of data points $\phi(U) \in \mathbb{R}^n$. By taking this functional view, a natural robustness measure for semivalue $\phi(\cdot,w)$ is its Lipschitz constant $L$, which is defined as the smallest constant such that

$$\|\phi(U;w) - \phi(\hat{U};w)\| \leq L \|U - \hat{U}\|$$

(115)

for all possible pairs of $U$ and $\hat{U}$.

**Theorem 18.** Among all semivalues, Banzhaf value ($w(k) = \frac{n}{2^n-1}$) achieves the smallest Lipschitz constant $L = \frac{1}{2^{n/2-1}}$. In other words, for Banzhaf value we have

$$\|\phi_{banz}(U) - \phi_{banz}(\hat{U};w)\| \leq \frac{1}{2^{n/2-1}} \|U - \hat{U}\|$$

(116)

for all possible pairs of $U$ and $\hat{U}$, and $L = \frac{1}{2^{n/2-1}}$ is the smallest constant among all semivalues.

**Proof.** Recall that a semivalue has the following representation

$$\phi_{\text{semi}}(i;U,w) := \frac{1}{n} \sum_{k=1}^{n} w(k) \sum_{S \subseteq N \setminus \{i\}, |S| = k-1} [U(S \cup i) - U(S)]$$

(117)

An interesting observation about semivalue is that the transformation $\phi : \mathbb{R}^{2^n} \to \mathbb{R}^n$ is always a linear transformation. Thus, for every semivalue, we can define *Semivalue matrix* $S_n \in \mathbb{R}^{n \times 2^n}$ where $\phi(U) = S_nU$. We denote the $i$th row of $S_n$ as $(S_n)_i$, and the entry in the $i$th row corresponding to subset $S$ as $(S_n)_{i,S}$. It is not hard to see that

$$(S_n)_{i,S} = \frac{1}{n} w(|S|) \text{ if } i \in S$$

(118)

$$(S_n)_{i,S} = -\frac{1}{n} w(|S| + 1) \text{ if } i \notin S$$

(119)

The Lipschitz constant of $\phi$ is thus equal to the operator norm of matrix $S_n$, which is the square root of the largest eigenvalue of matrix $S_nS_n^T$. Now we compute the eigenvalue of matrix $S_nS_n^T$.

For matrix $S_nS_n^T$, its diagonal entry is

$$d_1 = \sum_{S \in 2^n, |S| < n} \frac{1}{n^2} w^2(|S|) + \sum_{S \in 2^n, |S| < n} \frac{1}{n^2} w^2(|S| + 1)$$

(120)

$$= \frac{1}{n^2} \left[ \sum_{k=1}^{n} \left( \begin{array}{c} n-1 \cr k-1 \end{array} \right) w^2(k) + \sum_{k=1}^{n} \left( \begin{array}{c} n-1 \cr k-1 \end{array} \right) w^2(k) \right]$$

(121)

$$= \frac{2}{n^2} \sum_{k=1}^{n} \left( \begin{array}{c} n-1 \cr k-1 \end{array} \right) w^2(k)$$

(122)
and its non-diagonal entry is

\[
d_2 = \sum_{k=2}^{n} \binom{n-2}{k-2} \left( \frac{1}{n} w(k) \right)^2 + 2 \sum_{k=1}^{n-1} \binom{n-2}{k-1} \left( - \frac{1}{n^2} w(k) w(k+1) \right) + \sum_{k=0}^{n-2} \binom{n-2}{k} \left( \frac{1}{n} w(k+1) \right)^2
\]

(123)

\[
= \frac{1}{n^2} \sum_{k=0}^{n-2} \binom{n-2}{k} \left[ w^2(k+2) - 2w(k+1)w(k+2) + w^2(k+1) \right]
\]

(124)

\[
= \frac{1}{n^2} \sum_{k=0}^{n-2} \binom{n-2}{k} (w(k+2) - w(k+1))^2
\]

(125)

Therefore we can write \( S_n S_n^T = (d_1 - d_2) I_n + d_2 1_n \) where \( I_n \) is the identity matrix and \( 1_n \) is all-one matrix. The two eigenvalues are \( d_1 + (n-1)d_2 \) and \( d_1 - d_2 \). Since \( d_2 \geq 0 \), the top eigenvalue is \( d_1 + (n-1)d_2 \). Therefore, our goal is to find weight function \( w \) such that

\[
\min_w d_1 + (n-1)d_2
\]

subject to \( \sum_{k=1}^{n} \binom{n-1}{k-1} w(k) = n \)

(126)

(127)

that is, we want to solve

\[
\min_w \frac{2}{n^2} \sum_{k=1}^{n} \binom{n-1}{k-1} w(k)^2 + \frac{n-1}{n^2} \sum_{k=1}^{n-1} \binom{n-2}{k-1} (w(k) - w(k+1))^2
\]

subject to \( \sum_{k=1}^{n} \binom{n-1}{k-1} w(k) = n \)

(128)

(129)

Note that by Cauchy-Schwarz inequality,

\[
n^2 = \left( \sum_{k=1}^{n} \binom{n-1}{k-1} w(k) \right)^2
\]

(130)

\[
= \left( \sum_{k=1}^{n} \sqrt{\binom{n-1}{k-1} \binom{n-1}{k-1} w(k)^2} \right)^2
\]

(131)

\[
\leq \left( \sum_{k=1}^{n} \binom{n-1}{k-1} \right) \left( \sum_{k=1}^{n} \binom{n-1}{k-1} w(k)^2 \right)
\]

(132)

\[
= 2^{n-1} \sum_{k=1}^{n} \binom{n-1}{k-1} w(k)^2
\]

(133)

Thus the first term in the objective function is lower bounded by \( \frac{2}{n^2-1} \), which is achieved when \( w(1) = \ldots = w(n) = \frac{n}{2n-1} \), and this is also where the minimum of the second term achieved, i.e., just 0. Thus, the minimum possible \( \min_w = d_1 + (n-1)d_2 = \frac{1}{2n-1} \), and thus the operator norm of \( S_n = \sqrt{\frac{1}{2n-2}} = \frac{1}{\sqrt{n-1}} \).

\( \Box \)
C Experiment Settings & Additional Experimental Results

C.1 Implementation Details for Figure 1
We use MNIST dataset for Figure 1. For each given cardinality $k$, we sample 20 pairs of $(S, i)$ where $|S| = k$. For each sampled pair, we train 50 models on each of $S \cup i$ and $S$, i.e., we get 50 samples of $\text{acc}(A(S \cup i)) - \text{acc}(A(S))$. We then compute the estimate of $\text{SNR} = \frac{\mathbb{E}[|\text{acc}(A(S \cup i)) - \text{acc}(A(S))|]}{\text{std}(\text{acc}(A(S \cup i)) - \text{acc}(A(S)))}$ for each pair of $(S, i)$, and we compute the average SNR across all 20 pairs. For learning algorithm $A$, the “SmallCNN” refers to LeNet [LeCun et al., 1989] and the “Simple VGG” refers to a simplified VGG architecture. We use batch size 32, (initial) learning rate $10^{-3}$ and Adam optimizer for training.

We show additional results on CIFAR10 in Figure 5. For “Small CNN”, we refer to a small CNN model with two convolutional layers, followed by a max-pooling layer follows each with the ReLU as the activation function, and followed by three fully-connected layers. For “VGG11” we refers to VGG11 architecture [Simonyan and Zisserman, 2014]. As we can see from the figure, for all cardinalities, the average SNR for marginal contributions are $< 1$, and $\approx 0.20$ for most of the settings.

C.2 Settings for Figure 2
We estimate LOO, Shapley, and Banzhaf value on a size-2000 MNIST dataset. We use the state-of-the-art estimator for Shapley and Banzhaf value for Figure 2 (b) and (c): Permutation sampling for Shapley value and our MSR estimator for Banzhaf value. For both Shapley and Banzhaf value, we set the number of samples as 50,000. We compute the LOO with its exact formula but with noisy utility scores, and we align the number of (potentially repeated) samples also as 50,000. For each sample $S$, we train 5 models on it, obtain 5 noisy versions of $U(S)$, say $U_1, U_2, \ldots, U_5$. We then compute 5 different LOO/Shapley/Banzhaf values for 20 MNIST images, and compute the mean and variance of each value for each image, and draw the corresponding box-plot. The learning architecture we use is LeNet [LeCun et al., 1989], with batch size 32, (initial) learning rate $10^{-3}$ and Adam optimizer for training.

C.3 Details for Sample Efficiency Experiment in Section 5.1
For Figure 3 (a), we use a synthetic dataset with only 10 data points. To generate the synthetic dataset, we sample 10 data points from a bivariate Gaussian distribution where the means are 0.1 and $-0.1$ on each dimension, and covariance matrix is identity matrix. The labels are assigned to be the sign of the sum of the two features. The utility of a subset is the test accuracy of the model trained on the subset. A logistic regression classifier trained on the 10 data points achieves around 80% test accuracy. We show the Banzhaf value estimate for one data point in Figure 3 (a).
For Figure 3 (b), we use a size-500 MNIST dataset. The Relative Spearman Index is computed by the Spearman Index of the ranking of the value estimates between the current iteration, and the ranking of the value estimates when given additional 1000 samples. The learning architecture we use is LeNet [LeCun et al., 1989], with batch size 32, (initial) learning rate $10^{-3}$ and Adam optimizer for training.

### C.4 Details for Applications in Section 5.3

#### C.4.1 Datasets & Models

A comprehensive list of datasets and sources is summarized in Table 3. Similar to the existing data valuation literature [Ghorbani and Zou, 2019, Kwon and Zou, 2021, Jia et al., 2019b,c,a, Wang et al., 2020], we preprocess datasets for the ease of training. For Coverttype, Fraud, Creditcard, Vehicle, and all datasets from OpenML, we subsample the dataset to balance positive and negative labels. For these datasets, if they have multi-class, we binarize the label by considering $I[y = 1]$. For the image dataset CIFAR10, we follow the common procedure in prior works [Ghorbani and Zou, 2019, Jia et al., 2019b, Kwon and Zou, 2021]: we extract the penultimate layer outputs from the pre-trained ResNet18 [He et al., 2016]. The pre-training is done with the ImageNet dataset [Deng et al., 2009] and the weight is publicly available from PyTorch. We choose features from the class of Dog and Cat. The extracted outputs have dimension 512. For the image dataset MNIST and FMNIST, we directly train on the original data format, which is a more challenging setting compared with the previous literature.

For MNIST and FMNIST, we use LeNet [LeCun et al., 1989], with batch size 128, (initial) learning rate $10^{-3}$ and Adam optimizer for training. For CIFAR10 dataset, we use a two-layer MLP where there are 256 neurons in the hidden layer, with activation function ReLU, with batch size 128, (initial) learning rate $10^{-3}$ and Adam optimizer for training. For the rest of the datasets, we use a two-layer MLP where there are 100 neurons in the hidden layer, with activation function ReLU, with batch size 128, (initial) learning rate $10^{-2}$ and Adam optimizer for training. The logistic regression model for Coverttype dataset is adapted from Python module scikit-learn [Pedregosa et al., 2011],

| Dataset    | Source                                |
|------------|---------------------------------------|
| MNIST      | [LeCun, 1998]                         |
| FMNIST     | [Xiao et al., 2017]                   |
| CIFAR10    | [Krizhevsky et al., 2009]             |
| Click      | https://www.openml.org/d/1218         |
| Fraud      | [Dal Pozzolo et al., 2015]            |
| Creditcard | [Yeh and Lien, 2009]                  |
| Vehicle    | [Duarte and Hu, 2004]                 |
| Apsfail    | https://www.openml.org/d/41138        |
| Phoneme    | https://www.openml.org/d/1489         |
| Wind       | https://www.openml.org/d/847          |
| Pol        | https://www.openml.org/d/722          |
| CPU        | https://www.openml.org/d/761          |
| 2DPlanes   | https://www.openml.org/d/727          |
| Covertype  | [Blackard, 1998]                     |

Table 3: A summary of datasets used in Section 5.3’s experiments.
with ‘liblinear’ solver. The training of logistic regression on Covertype dataset does not involve randomness.

C.4.2 Experiment Settings

For both tasks, we consider 200 and 2000 samples as validation dataset and hold-out test set. The validation dataset is used to estimate utility, and all the results are based on this held-out dataset. For MNIST, FMNIST, and CIFAR10, we consider the number of data points being valued as 2000. For Click dataset, we consider the number of data points being valued as 1000. For the rest of the datasets, we consider the number of data points being valued as 200. For each data value we show in Table 1 and 2, we use the corresponding state-of-the-art estimator to estimate them (for Data Shapley, we use Permutation Sampling; for Data Banzhaf, we use our MSR estimator; for Beta Shapley, we use the Monte Carlo estimator by [Kwon and Zou, 2021]). We stress that the Monte Carlo estimator by [Kwon and Zou, 2021] is not numerically stable when the training set size $>500$, so for datasets with $>500$ data points (MNIST, FMNIST, CIFAR10, and Click), we omit the results for Beta Shapley. We set the number of samples to estimate Data Banzhaf, Data Shapley, and Beta Shapley as 100,000.

All of our experiments are performed on Tesla P100-PCIE-16GB GPU.

**Learning with Weighted Samples.** For each estimated data value, we normalize it to $[0, 1]$ by $\frac{\text{value} - \min}{\max - \min}$. Let $\phi(i)$ be the normalized value for data point $i$. We compare the test accuracy of a weighted risk minimizer $f_\phi$ defined as

$$f_\phi := \arg\min_f \sum_{i \in N} \phi(i)\text{loss}_f(i)$$

(134)

where $\text{loss}_f(i)$ denote the loss of $f$ on data point $i \in N$.

**Noisy Label Detection.** We flip 10% of the labels by picking an alternative label from the rest of the classes uniformly at random.

C.5 Details and Additional Results for Rank Stability in Appendix 5.2

In this section, we describe the detailed settings and additional results on comparing the rank stability of different data values on a natural dataset and natural learning stochasticity. We also compare with the least cores, another existing data value notion which is not a semivalue but also originates from cooperative game theory (see the description in Related Work A). The estimation algorithms for the least core is the Monte Carlo algorithm from [Yan and Procaccia, 2020].

**Settings.** We experiment on ‘CPU’ (200 data points) and ‘CIFAR10’ (500 data points) datasets from Table 3. In this case, we cannot compute the exact data values. The data preprocessing procedure, model training hyperparameters, and the estimation algorithm for semivalues are the same as what are described in Appendix C.4.1 and C.4.2. The perturbations of the model performance scores are caused by the randomness in neural network initialization and mini-batch selection.

The tricky part in the experiment design is that we need to find a way to adjust the scale of the perturbation caused by a natural stochastic learning algorithm. Our preliminary experiments show that the variance of performance scores does not have a clear dependency on the training...
hyperparameters such as mini-batch sizes. To solve this challenge, we design the following procedure to control the magnitude of the perturbation with a single parameter $k$:

1. Sample $m$ data subsets $S_1, \ldots, S_m$ (the sampling strategy varying for specific semivalue estimators).

2. For each subset $S_i$, we execute $\hat{U}(S_i)$ for $k$ times and obtain $k$ independent performance score samples $u_1, \ldots, u_k \sim \hat{U}(S_i)$. We compute $\tilde{U}_k(S_i) = \frac{1}{k} \sum_{j=1}^{k} u_j$.

3. Estimate the semivalue with the corresponding estimators based on samples $\tilde{U}_k(S_1), \ldots, \tilde{U}_k(S_m)$.

Essentially, $k$ is the number of rounds that we run a stochastic learning algorithm in order to estimate the expected utility on a given subset. With larger $k$, the noise in the estimated utility will become smaller. Since it is infeasible to compute the groundtruth data values for this experiment, we approximate the groundtruth by setting $k = 50$. Intuitively, as $k$ increases, the difference between $\hat{U}_k(S_i)$ and the approximated groundtruth scores will be smaller with high probability. We set the budget of samples used to estimate the semivalues as $m = 2000$ (same for the groundtruth) for all semivalues for fair comparison. It is worth noting that in this case, the rank stability is not just related to the property of the data value notion, but also the corresponding estimator.

Results. We plot the Spearman index between the approximated groundtruth data value ranking and the estimated data value ranking with different $k$s. The results are shown in Figure 6. As we can see, Data Banzhaf once again outperforms all other data value notions, and achieves a better rank stability than others by a large margin for a wide range of $k$’s.

C.6 Additional Results for Ranking Preservation Experiment without Estimators

The ranking preservation results in Section 5.2 and Appendix C.5 do not compute the exact data value but use the corresponding estimation algorithms. In this Section, we present an additional result on ranking preservation when we are able to compute the exact data value. Similar to the evaluation protocol for sample efficiency comparison, we additionally experiment on a synthetic dataset with a scale (10 data points) that we can compute the exact ranking for different data value
Figure 7: Impact of the noise in utility scores on the stability of data value ranking measured by Spearman index between the ranking of exact data value and the ranking of data value estimated from noisy utility scores.

specifically, we use the same synthetic dataset as in the sample efficiency experiment in section 5.1. The performance score of a subset is the test accuracy of the Logistic regression model trained on the subset. In figure 7, we plot the Spearman index between the ranking of exact data values and the ranking of data values computed from noisy utility scores. For each noise scale $\sigma$ on the x-axis of figure 7 (a), we add random Gaussian noise $\mathcal{N}(0, \sigma I)$ to perturb the performance score. That is, $\hat{U} = U + \mathcal{N}(0, \sigma I)$. We then compute the Spearman index between the ranking of exact data values (derived from $U$) and the ranking of data values derived from noisy utility scores $\hat{U}$. We repeat this procedure for 20 times and take the average Spearman index for each point in the figure.

The main considerations behind the design choices of synthetic dataset and Gaussian noise addition are the following:

- In order to rule out the influence of estimation error, we would like to compute the exact ranking of data points in terms of different data value notions, which means that we can only use a toy example with $\leq 15$ data points. In this case, it does not make sense to use SGD for training.
- According to our preliminary experiment results, the variance of performance scores does not have a clear dependency on the SGD's training hyperparameters such as mini-batch sizes. The relationship between performance variance and training hyperparameters is an interesting direction for future work.

C.7 Additional Results for Rank Stability on Gradient Descent with Randomized Smoothing

In our experiment, we mainly use SGD and its variants as the test case since SGD is arguably the most frequently used stochastic learning algorithms nowadays. However, the robustness guarantee derived in our theory (section 4) is agnostic to the structure of perturbation, which means that it applies to perturbations caused by arbitrary kinds of learning algorithms. Therefore, we expect to get similar rank stability results when experimenting with other kinds of stochastic learning algorithms. For completeness, we perform an additional ranking preservation experiment with another useful stochastic learning algorithm, gradient descent with randomized smoothing Duchi et al. [2012].
Figure 8: The stability of data value ranking measured by Spearman index between the ranking of “groundtruth” data value and the ranking of data value estimated from noisy utility scores, where (a) is on CPU dataset and (b) is on CIFAR10 dataset.

We use \( \text{loss}(\theta, N) = \sum_{i \in N} \text{loss}(\theta, i) \) to denote the loss of model with parameter \( \theta \) on the dataset \( N \). For regular gradient descent, at iteration \( t \), the model is updated as

\[
\theta_{t+1} = \theta_t - \eta \nabla \text{loss}(\theta_t, N)
\]  

where \( \nabla \) denotes the derivative with respect to \( \theta \). In contrast to the regular gradient descent, randomized smoothing technique convolves Gaussian noise with the original learning loss function and the model is updated instead by “smoothed gradient”:

\[
\theta_{t+1} = \theta_t - \eta \frac{1}{\ell} \sum_{j=1}^{\ell} \nabla \text{loss}(\theta_t + \alpha \mathcal{N}(0, \mathbf{I}), N)
\]

We compare the rank stability of different semivalues on the CPU dataset and the CIFAR10 dataset, with the exactly the same experiment setting as in Appendix C.5, except for replacing SGD-based training with the gradient descent with randomized smoothing technique. We set \( \ell = 1 \) to introduce larger randomness, and the smoothing radius \( \alpha \) to be equal to the learning rate. The results are shown in Figure 8. As we can see, Data Banzhaf once again outperforms all other data value notions when the sources of performance score perturbation are changed from SGD to gradient descent with randomized smoothing.