Efficient Computation and Analysis of Distributional Shapley Values

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Abstract

Distributional data Shapley value (DShapley) has been recently proposed as a principled framework to quantify the contribution of individual datum in machine learning. DShapley develops the foundational game theory concept of Shapley values into a statistical framework and can be applied to identify data points that are useful (or harmful) to a learning algorithm. Estimating DShapley is computationally expensive, however, and this can be a major challenge to using it in practice. Moreover, there has been little mathematical analyses of how this value depends on data characteristics. In this paper, we derive the first analytic expressions for DShapley for the canonical problems of linear regression and non-parametric density estimation. These analytic forms provide new algorithms to compute DShapley that are several orders of magnitude faster than previous state-of-the-art. Furthermore, our formulas are directly interpretable and provide quantitative insights into how the value varies for different types of data. We demonstrate the efficacy of our DShapley approach on multiple real and synthetic datasets.

1 Introduction

Data valuation has emerged as an important topic for machine learning (ML) as well as for the broader discussions around the economics of data. Proposed policies such as the Dashboard Act and data dividend in the US would stipulate that companies need to quantify the value of the data that they collect from users [33]. Such valuation could have important implications for policy, regulation, taxation and potentially even for individual compensation [29]. Recently data Shapley, a data valuation framework based on the foundational Shapley value in economics, has gained significant attention [15][22]. Data Shapley is appealing from a policy perspective because it inherits the same fair allocation properties that the original Shapley value uniquely satisfies. Moreover, it has shown to empirically capture the notion of which training data helps or harms the ML model.

A fundamental limitation of data Shapley, however, is that it is defined with respect to a fixed dataset. The statistical and random nature of data is ignored. Accordingly, data Shapley needs to be recalculated even when the dataset changes slightly, which is computationally expensive, and it could also be unstable for randomly drawn datasets. To tackle these challenges, Ghorbani et al. [14] proposed distributional Shapley value (DShapley) as the natural statistical extension of the Shapley value, by considering the expected value of data Shapley value with respect to the underlying distribution. While DShapley is numerically more stable and does not require the aforementioned recalculation, DShapley is still mathematically challenging to analyze and computationally hard to estimate.

In this paper, we address these challenges by developing rigorous analyses and computationally efficient algorithms for DShapley. Theoretical contribution: we develop the first analytic expres-
We review existing Shapley value-based data valuation methods. To begin with, we define some
work, the only efficient analytic form for data Shapley is just for the nearest neighbor classifier [21];
which is several orders of magnitude faster than previous state-of-the-art. We support our analyses
(1) uniquely satisfies the natural properties of fair valuation: symmetry, null player, and additivity
The original data Shapley value is defined with respect to a fixed dataset
These approaches lack the the fairness principles that has uniquely satisfied by the Shapley value.
value (1) in the Supplementary Material.
example, in the classification problem, \( U \) could be the test accuracy of a model trained using a subset \( S \).
In supervised learning, we set \( Z = (X, Y) \), where \( X \) and \( Y \) are the input and its label, respectively,
and in unsupervised learning \( Z = X \). We denote a utility function \( U \) by \( U: \cup_{j=0}^{\infty} Z^j \rightarrow \mathbb{R} \). Here, we
use the conventions \( Z^0 := \{\emptyset\} \) and \( U(\emptyset) = 0 \). For a set \( S \), we denote its cardinality by \( |S| \), and we
use \([m]\) to denote a set of integers \( \{1, \ldots, m\} \).

Data Shapley value applies the cooperative game theory concept of Shapley value to ML problems
[15,22]. More precisely, given a utility function \( U \) and a fixed dataset \( B \subseteq Z \) with \( |B| = m \), data
Shapley value of a point \( z^* \in B \) is defined as
\[
\phi(z^*; U, B) := \frac{1}{m} \sum_{j=1}^{m} \frac{1}{(m-1)!} \sum_{S \in B \setminus z^*, j} (U(S \cup \{z^*\}) - U(S)),
\]
where \( B \setminus z^* := \{S \subseteq B \setminus \{z^*\} : |S| = j - 1\} \) for \( j \in \mathbb{N} \). The cardinality \( |B_j \setminus z^*| \) is \( \binom{m-1}{j-1} \) for all
\( j \in [m] \), meaning that data Shapley value (1) is a weighted average of the marginal contribution
of \( z^* \) to each \( S \subseteq B \). Data Shapley provides a principled data valuation regime in that the value
(1) uniquely satisfies the natural properties of fair valuation: symmetry, null player, and additivity
[15,21]. We review the detailed information on these properties and the uniqueness of data Shapley
value (1) in the Supplementary Material.

The original data Shapley value is defined with respect to a fixed dataset \( B \). Even if a single point in
\( B \) is changed, in principle, all of the values should be recomputed. This is particularly problematic
in typical statistics and ML settings, where the data points are samples from an underlying distribution.
In order to capture the statistical nature of data valuation, DShapley was recently proposed where
data Shapley is treated as a random variable [14]. To be more specific, given a utility function \( U \), a
data distribution \( P_Z \), and some \( m \in \mathbb{N} \), Ghorbani et al. [14] defined DShapley of a point \( z^* \) as
\[
\nu(z^*; U, P_Z, m) := \mathbb{E}_{B \sim P_Z^m} [\phi(z^*; U, B \cup \{z^*\})].
\]
DShapley [2] is the expectation of data Shapley value (1) over random datasets of size \( m \) containing
\( z^* \). Ghorbani et al. [14] further showed that DShapley possesses some desirable properties. For

1The function \( U \) is also known as a potential function or a performance metric in other literature. For example, in the classification problem, \( U(S) \) could be the test accuracy of a model trained using a subset \( S \).
instance, DShapley is stable under small perturbations to the data points themselves and to the underlying data distribution, which have not been clear with (1). However, estimating DShapley is often computationally expensive and thus it critically hampers the practical use of DShapley. In this paper, we focus on canonical problems of linear regression and non-parametric density estimation, deriving new expressions for DShapley that lead to new mathematical insights and efficient computation algorithms.

3 Distributional Shapley values for linear regression

We present rigorous analyses of DShapley for linear regression problems. In Sec. 3.1, we first provide a general reformulation of DShapley without distributional assumptions on inputs. In Sec. 3.2, we simplify DShapley as a function of Mahalanobis distance and an error when inputs are Gaussian. In Sec. 3.3, we provide upper and lower bounds for DShapley when inputs are sub-Gaussian.

3.1 A general reformulation of distributional Shapley values

Throughout this section, we let \((X,Y)\) be a pair of input and output random variables defined on \(\mathcal{X} \times \mathcal{Y} \subseteq \mathbb{R}^p \times \mathbb{R}\). We assume that \(Y = X^T \beta + \varepsilon\) is the underlying linear model where \(\varepsilon\) is a random error whose mean is zero and variance is \(\sigma^2\). Here, \(X\) can come from an arbitrary distribution with bounded first two moments. For a subset \(S \subseteq \mathcal{X}\), we denote a design matrix and its corresponding output vector based on \(S\) by \(X_S \in \mathbb{R}^{|S| \times p}\) and \(Y_S \in \mathbb{R}^{|S|}\), respectively.

For \(\gamma \geq 0\), the ridge regression estimator based on \(S\) is defined as \(\hat{\beta}_{S,\gamma} := (X_S^T X_S + \gamma I_p)^{-1} X_S^T Y_S\) where \(I_p\) is the \(p \times p\) identity matrix. For \(q \in \mathbb{N}\), we consider a utility function \(U_{q,\gamma}(S) := (C_{lin} - \int (y - x^T \hat{\beta}_{S,\gamma})^2 dP_{X,Y}(x,y)) \mathbb{1}(|S| \geq q)\) where \(C_{lin}\) is some fixed constant and \(\mathbb{1}(\cdot)\) is the indicator function. We denote the Gaussian distribution with mean \(\mu\) and covariance \(\Sigma\) by \(\mathcal{N}(\mu, \Sigma)\).

Lastly, we denote the data to be valued by \((x^*, y^*)\) and its error by \(e^* := y^* - x^{*T} \beta\).

The DShapley can be equivalently expressed as follows [12]:

\[
\nu((x^*, y^*); U_{q,\gamma}, P_{X,Y}, m) = \mathbb{E}_{j \sim [m]} \mathbb{E}_{S \sim P_X} [U_{q,\gamma}(S \cup \{(x^*, y^*)\})] - U_{q,\gamma}(S), \tag{3}
\]

where \(j \sim [m]\) denotes \(j\) follows a uniform distribution over \([m]\). Using Equation (3), we further derive a general reformulation of DShapley in the following proposition.

**Proposition 1 (A general form of DShapley).** Let \(\mathbb{E}[Y \mid X] = X^T \beta\), \(\text{Var}(Y \mid X) = \sigma^2\), and \(\mathbb{E}(XX^T) = \Sigma_X\). Then, for any \(q \geq 2\) and some fixed constant \(C_{lin}\), DShapley of a point \((x^*, y^*) \in \mathcal{X} \times \mathcal{Y}\) with the ridge regression estimator is given by

\[
\nu((x^*, y^*); U_{q,\lambda}, P_{X,Y}, m) = \frac{1}{m} \sum_{j=1}^{m} \mathbb{E}_{X \sim P_X} \mathbb{E}_{S \sim P_X} \left[ x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} x^* \left(1 + x^T A_{S,\gamma}^{-1} x^* \right)^{-2} \right] + h(\gamma),
\]

where \(A_{S,\gamma}^{-1} := (X_S^T X_S + \gamma I_p)^{-1}\) and \(h(\gamma)\) is a term such that \(\lim_{\gamma \to 0^+} h(\gamma) = 0\) and \(h(0) = 0\).

The implication of different choice of the constant \(C_{lin}\)  By the expression (3), different choice of the constant \(C_{lin}\) in the utility function \(U_{q,\gamma}\) causes constant changes in DShapley. To be more specific, for \(C \in \mathbb{R}\), if \(U_{q,\gamma} = \hat{U}_{q,\gamma} + C\), then \(\nu((x^*, y^*); U_{q,\lambda}, P_{X,Y}, m) = \nu((x^*, y^*); \hat{U}_{q,\lambda}, P_{X,Y}, m) + C/m\). In this respect, we simply choose a constant \(C_{lin}\) that gives the simplest form in Proposition 1 and the following results.

Proposition 1 simplifies the expected value of the marginal contributions of \((x^*, y^*)\) in Equation (3) with a few terms such as the label error \(e^*\) and the ridge leverage score \(x^* A_{S,\gamma}^{-1} x^*\) [25]. This new formulation provides mathematical insights and interpretations. For instance, for fixed \(x^*\), DShapley is negatively related to the label error \(e^*\) as long as \(\gamma\) is small enough; as the error decreases, DShapley increases. In addition, DShapley is determined only by the first two conditional moments of \(Y\) given \(X\), meaning that it does not rely on other higher moments or a particular distribution of \(Y\). Furthermore, it is noteworthy that Proposition 1 does not require a specific distributional assumption on \(X\) except for the moment condition \(\mathbb{E}(XX^T) = \Sigma_X\). In the following sections, we pay more attention to the input distribution and propose computationally efficient algorithms for DShapley.
3.2 Distributional Shapley value under Gaussian inputs

If the data come from a Gaussian distribution, we can derive a simpler expression for DShapley.

**Theorem 2** (DShapley under Gaussian inputs). Assume $\mathbb{E}[Y \mid X] = X^T \beta$, $\text{Var}(Y \mid X) = \sigma^2$ and $X \sim \mathcal{N}_p(0, \Sigma_X)$. For $k \geq p$, we denote a Chi-squared distribution with degree of freedom $k - p + 1$ by $T_k$, i.e., $T_k \sim \chi^2_{k-p+1}$. Then, for any $q \geq p + 3$ and some fixed constant $C_{\text{lin}}$, DShapley of a point $(x^*, y^*) \in \mathcal{X} \times \mathcal{Y}$ with the least square estimator is given by

$$
\nu((x^*, y^*); U_{q,0}, P_{X,Y}, m) = -\frac{1}{m} \sum_{j=q}^{m} \mathbb{E} \left[ j - 1 \left( x^* x_j^{-1} x^* + T_j \sigma^2 \right) \right].
$$

where the expectation is with respect to the Chi-squared distributions.

**Theorem 2** presents a simple representation of DShapley when $\gamma = 0$ and inputs are Gaussian. The new form depends only on the two terms, the error $e^*$ and the term $x^* \Sigma^{-1} x^*$, also known as the Mahalanobis distance of $x^*$ from zero with respect to $\Sigma_X$. A direct implication of (4) is that any points with the same error level have the same DShapley when they have the same Mahalanobis distance. Similar to Proposition 4, a role of $e^2$ is also explicitly explained. Suppose there are two points with the same inputs but different error levels, i.e., $(x^*, y_1^*)$ and $(x^*, y_2^*)$ such that $e_1^2 > e_2^2$. Then, DShapley for the point with the smaller error is higher than the other point, i.e., $\nu((x^*, y_1^*)_{U_{q,0}}, P_{X,Y}, m) \leq \nu((x^*, y_2^*)_{U_{q,0}}, P_{X,Y}, m)$. This inequality matches our intuitions that the big error $e^2$ is likely to produce small marginal contributions $U_{q,0}(S \cup \{(x^*, y^*)\}) - U_{q,0}(S)$.

**Estimation of DShapley** As for the estimation of DShapley $\nu((x^*, y^*); U_{q,0}, P_{X,Y}, m)$, we exploit the Monte-Carlo approximation method. DShapley can be viewed as a cumulative sum of decreasing elements, so it might be computationally inefficient to compute every expectation term. Instead of computing the cumulative sum, we consider the partial sum by ignoring negligible expectation terms. We describe a simple version of the proposed algorithm in Algorithm 1. Detailed version is provided in the Supplementary Material.

A similar idea has been suggested in a number of algorithms including TMC-SHAPLEY [15] or D-SHAPLEY [14]. Although the previous state-of-the-art algorithms and the proposed algorithm make use of the Monte-Carlo method, there are notable differences. Since the previous algorithms require to evaluate the utility function $U_{q,0}(S)$ for each random sample of $S$, they need to compute the matrix inversion $(X_S^T X_S)^{-1}$ at every iteration. Hence, when the maximum number of Monte-Carlo samples is $T$, the computational complexity of the previous state-of-the-art algorithms is $O(m T^3)$. However, the proposed Algorithm 1 only needs to perform the matrix inversion once for $\Sigma_X^{-1}$, and the computational complexity for the proposed algorithm is $O(m T + p^3)$, which is substantially smaller than $T$ is usually large. Also, all the previous algorithms might be unstable if the cardinality of a random set $|S|$ is not much bigger than $p$, but the proposed algorithm does not require such matrix inversion steps.

**Illustration of DShapley** To see how DShapley changes with respect to $x^* \Sigma^{-1} x^*$ and $e^2$, we estimate DShapley using Algorithm 1. We consider $m \in \{100, 300, 500\}$, $e^2 \in \{0, 1, 2, 4, 8\}$, the Gaussian input distribution $X \sim \mathcal{N}_p(0, I_p)$ with $p = 10$, and the utility hyperparameter $q = p + 10$. Here, we assume that $\Sigma_X^{-1}$ and $e^2$ are given. Figure 1 illustrates DShapley as a function of $x^* \Sigma^{-1} x^*$. As anticipated, for a fixed $x^* \Sigma^{-1} x^*$, DShapley decreases as $e^2$ increases. Note that DShapley exhibits different behavior depending on the error level. When $e^2$ is small, DShapley increases as $x^* \Sigma^{-1} x^*$ increases. However, when $e^2$ is big, DShapley shows U-shape curve. This is because of its form (4); it mainly relies on $e^2$ for small values of $x^* \Sigma^{-1} x^*$ and it converges to zero as $x^* \Sigma^{-1} x^*$ diverges. Note that the fraction in (4) has a form of a weighted sum of $e^2$ and $\sigma^2$. Lastly, the absolute magnitude of DShapley gets smaller as $m$ increases. Additional results when $p = 30$ are provided in the Supplementary Material.

3.3 Distributional Shapley values under sub-Gaussian inputs

In this section, we develop closed-form bounds for DShapley when inputs are sub-Gaussian. To be more formal, we first define the sub-Gaussian.
Algorithm 1: DShapley for the least square estimator under Gaussian inputs.

Require: A true value or an estimate for \( x^* x^T \Sigma_X^{-1} x^* \), \( e^2 \), and \( \sigma^2 \). The maximum number of Monte Carlo samples \( T \). A utility hyperparameter \( q \geq p + 3 \).

procedure
\[ \text{for } j \in \{1, \ldots, m\} \text{ do} \]
\[ \text{for } i \in \{1, \ldots, T\} \text{ do} \]
\[ \text{Sample } t_{i[j]} \text{ from the } \chi^2_{p+1}. \]
\[ A_j \leftarrow \left( \frac{i - 1}{A_j + \frac{1}{i-p} \frac{x^T \Sigma_X^{-1} x^* e^2 + t_{i[j]} \sigma^2}{x^T \Sigma_X^{-1} x^* + t_{i[j]} \sigma^2}} \right) / i \]
\[ \text{end for} \]
\[ \hat{\nu} \leftarrow \hat{\nu} - A_j / m \]
\[ \text{end for} \]
\[ \hat{\nu}(x^*, y^*); U_q, P_{X,Y}, m) \leftarrow \hat{\nu} \]
\[ \triangleright \text{Estimates for DShapley} \]
\[ \text{end procedure} \]

Figure 1: The illustration of DShapley as a function of the Mahalanobis distance \( x^T \Sigma_X^{-1} x^* \). Different colors indicate different error levels.

Definition 1 (Sub-Gaussian). We say that a random variable \( X \) in \( \mathbb{R} \) is sub-Gaussian if there are constants \( C_{\text{sub}} \) and \( \nu_{\text{sub}} \) such that for every \( t > 0 \), \( P(|X| > t) \leq C_{\text{sub}} e^{-\nu_{\text{sub}} t^2} \) holds. In addition, we say that a random vector \( X \) in \( \mathbb{R}^p \) is sub-Gaussian if the one-dimensional marginals \( \langle X, x \rangle \) are sub-Gaussian random variables for all \( x \in \mathbb{R}^p \).

Note that a class of sub-Gaussian includes many useful random variables such as Gaussian and any bounded random variables [32]. Now we develop bounds for DShapley in the following theorem.

Theorem 3 (Upper and lower bounds for DShapley under sub-Gaussian inputs). Assume that \( E[Y \mid X] = X^T \beta \) and \( \text{Var}(Y \mid X) = \sigma^2 \). Suppose \( Y \) is bounded and \( X \) are mean zero sub-Gaussian in \( \mathbb{R}^p \) with \( E(X X^T) = \Sigma_X \). Then, for \( q \geq 2 \) and some fixed constant \( C_{\text{lin}} \), DShapley of a point \( (x^*, y^* \in \mathcal{X} \times \mathcal{Y} \) with the ridge regression estimator has the following bounds.

\[
\frac{1}{m} \sum_{j=q-1}^{m-1} \frac{x^T \Sigma_X^{-1} x^* \Lambda_{\text{lower}}^2(j)}{(1 + x^T \Sigma_X^{-1} x^* \Lambda_{\text{upper}}(j))^2} \left( 2 + x^T \Sigma_X^{-1} x^* \Lambda_{\text{lower}}(j) \right) \sigma^2 - \Lambda_{\text{ratio}}(j)e^2 \right) + o \left( \frac{1}{m} \right)
\]

\[
\leq \nu((x^*, y^*); U_q, \gamma, P_{X,Y}, m) - h(\gamma)
\]

\[
\leq \frac{1}{m} \sum_{j=q-1}^{m-1} \frac{x^T \Sigma_X^{-1} x^* \Lambda_{\text{upper}}^2(j)}{(1 + x^T \Sigma_X^{-1} x^* \Lambda_{\text{lower}}(j))^2} \left( 2 + x^T \Sigma_X^{-1} x^* \Lambda_{\text{upper}}(j) \right) \sigma^2 - \Lambda_{\text{ratio}}(j)e^2 \right) + o \left( \frac{1}{m} \right),
\]

where the term \( h \) is defined in Proposition 7 and

\[
\Lambda_{\text{ratio}}(j) = \left( 1 + x^T \Sigma_X^{-1} x^* \Lambda_{\text{lower}}(j) \right) \left( 1 + x^T \Sigma_X^{-1} x^* \Lambda_{\text{upper}}(j) \right)^2,
\]

\( \Lambda_{\text{lower}}(j) \) and \( \Lambda_{\text{upper}}(j) \) are two explicit constants that scale \( O(1/j) \) and depend only on \( \gamma \) and the sub-Gaussian distribution. The explicit expression for \( \Lambda_{\text{lower}}(j) \) and \( \Lambda_{\text{upper}}(j) \) are provided in the Supplementary Material.

Theorem 3 provides upper and lower bounds for DShapley when inputs are sub-Gaussian. As Theorem 2 the main component of the bounds consists of the Mahalanobis distance \( x^T \Sigma_X^{-1} x^* \) and
the error $e^{r^2}$. Hence, data points with the same Mahalanobis distance have the same DShapley if the error levels are the same. Although the new bounds in Theorem 3 are not the exact form of DShapley, they are analytically expressed, and can be efficiently computed without Monte Carlo sampling.

**The two assumptions in Theorem 3** Compared to Proposition 1, we additionally assume the boundness of $\mathcal{Y}$ and the sub-Gaussian distribution on inputs in Theorem 3. The former implies the boundness of the marginal contribution $U_{q,n}(S \cup \{(x^*, y^*)\}) - U_{q,n}(S)$, and the latter ensures that eigenvalues of $A^{-1}_{S,n}$ are in $[\Lambda_{\text{lower}}(j), \Lambda_{\text{upper}}(j)]$ with high probability. Combining these two ingredients, we obtain the bounds for DShapley as a function of $\Lambda_{\text{lower}}(j)$ and $\Lambda_{\text{upper}}(j)$.

### 4 Distributional Shapley values for non-parametric density estimation

In this section, we study DShapley for non-parametric density estimation problems. We let $Z$ be a random variable defined on $Z \subseteq \mathbb{R}^d$ as in Sec. 2 and let $p(z)$ be the underlying probability density function. We consider the kernel density estimator (KDE), a fundamental non-parametric density estimator in statistics [30, 28]. For a kernel function $k : Z \to \mathbb{R}$, the KDE based on a dataset $S \subseteq Z$ is denoted by $\hat{p}_{S,k}(z) = \frac{1}{|S|} \sum_{i \in S} k(z - z_i)$. By convention, we assume that a kernel is bounded and parameterized by a bandwidth $h > 0$, i.e., $k_h(\cdot) := h^{-d} k(\cdot / h)$ for a kernel $k$. For notational convenience, we suppress the bandwidth notation and use $k$ instead of $k_h$. We consider a utility function by $U_k(S) = \hat{C}_{\text{den}} - \int (p(z) - \hat{p}_{S,k}(z))^2 dz I(|S| \geq 1)$ where $C_{\text{den}}$ is some constant. As before, changing the constant $C_{\text{den}}$ simply shifts the value of all the points by the same constant; therefore we just set $C_{\text{den}}$ to simplify expressions of DShapley.

Before going to the analysis, we define DShapley of a set, a natural extension of DShapley of a point, by regarding a set as a point. More precisely, given a utility function $U$, a data distribution $P_Z$, and some $m \in \mathbb{N}$, we define DShapley of a set as follows.

$$
\nu(S' ; U, P_Z, m) := \mathbb{E}_{j \sim [m]} \mathbb{E}_{S \sim P_Z^m} [U(S \cup S') - U(S)].
$$

**Theorem 4 (DShapley for non-parametric density estimation),** Let $S^* \subseteq Z$ be a set to be valued such that $|S^*| = n$. Then, for some fixed constant $C_{\text{den}}$, DShapley of $S^*$ with the KDE is given by

$$
\nu(S^* ; U_k, P_Z, m) = -A(n, m) \int (p(z) - \hat{p}_{S^*,k}(z))^2 dz + B(n, m) g(S^*),
$$

where $g(S^*) := \int \hat{p}_{S^*,k}(z) (p(z) - \mathbb{E}[k(z-Z)]) dz$.

**The term $g(S^*)** Suppose $p(z)$ is twice continuously differentiable and a kernel $k$ is continuous and has a compact support. Then the bias $(p(z) - \mathbb{E}[k(z-Z)])$ of the KDE is $O(h^2)$ and thus $g(S^*) = O(h^2)$ [16 Equation (1.131)].

**Theorem 4** shows the exact form of DShapley of a set $S^*$. As discussed above, under the mild conditions, the second term is $O(h^2)$, so we focus on the first term. The first term is the negative constant $-A(n, m)$ times to the integrated squared error (ISE) of $\hat{p}_{S^*,k}$. That means, DShapley of a set $S^*$ increases as ISE decreases, and vice versa. Note that the ISE could be interpreted as performance of $S^*$. In the following examples, we provide more insights on DShapley based on Theorem 4.

**Example 1 (A set with two elements).** Suppose $S^* = \{z^*_1, z^*_2\}$, $p(z) = 1$ for all $z \in [0, 1]$ and $k(z - z_i) = \frac{1}{2} I(\left\{\frac{z - z_i}{h} \right\} \leq \frac{1}{2})$. We set a bandwidth such that $h \leq 2 \min\{z^*_1, z^*_2, (1 - z^*_1), (1 - z^*_2)\}$.

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2 We define a kernel function as follows. For a non-negative function $k : Z \to \mathbb{R}$, we say $k$ is a kernel if $\int k(z) dz = 1$ and $k(z) = k(-z)$ for all $z \in Z$.

1 A weaker condition for the $O(h^2)$-bias statement is as follows. For all $i \in [d]$, a kernel satisfies $\int z_{i1} k(z) dz < \infty$ and $\int |z_{i1}|^2 k(z) dz < \infty$ where $z = (z_{i1}, \ldots, z_{id}) \in \mathbb{R}^d$. Many useful kernels such as the Gaussian kernel satisfy the condition [16].
Then, we have a closed-form expression for DShapley as follows.

\[ \nu(S^*; U, P_Z, m) = \begin{cases} A(2, m) \left( 1 - \frac{1}{2\pi} \right) + C_{set} & \text{if } \Delta \geq h, \\ A(2, m) \left( 1 - \frac{1}{h} + \frac{\Delta}{2\pi p} \right) + C_{set} & \text{if } \Delta < h, \end{cases} \]

where \( \Delta := |z_1^* - z_2^*| \) and \( C_{set} \) is some explicit constant independent of \( S^* \). It is noteworthy that DShapley for a set satisfying \( \Delta < h \) is less than the value of a set with \( \Delta \geq h \), due to \( \frac{\Delta}{2\pi p} < \frac{1}{\sqrt{\pi}} \). In other words, for fixed \( h \), if the two data points are farther than \( h \), DShapley gets larger.

**Example 2** (Synergy of two elements). We suppose the same setting with Example 7 and now investigate the case where DShapley of \( S^* \) is greater than the sum of two DShapleys of the point, i.e.,

\[ \nu(\{z_1^*, z_2^*\}; U, P_Z, m) \geq \nu(z_1^*; U, P_Z, m) + \nu(z_2^*; U, P_Z, m). \]  

We say there is a synergy of \( z_1^* \) and \( z_2^* \) when the inequality \( (5) \) holds. Although a similar analysis used in Example 7 gives \( \nu(z_1^*; U, P_Z, m) \) a closed-form expression, it is difficult to know when \( (5) \) holds analytically. We empirically show that for fixed \( h \), synergy happens when \( \Delta \) is bigger than some threshold. Detailed information for Examples 1 and 2 is available in the Supplementary Material.

## 5 Numerical experiments

We now demonstrate the practical efficacy of the DShapley using synthetic and real datasets. Implementation details and Python scripts are available in the Supplementary Material.

### Comparison of the computational time

We first compare the computational time of D-SHAPLEY by Ghorbani et al. [14] with Algorithm 1 in linear regression settings. As we mentioned in Sec. 3.2, the existing algorithm requires the utility function evaluation, and thus it is anticipated to have heavier computational costs than the proposed algorithm.

Table 1 shows the computational time of state-of-the-art D-SHAPLEY and Algorithm 1 in various \((m, p)\). We use the Gaussian synthetic datasets used in Figure 1. The computational time is measured with the one Intel® Xeon® E7-8867v4 processor. In all cases, the proposed algorithm is at least about 11 times faster than D-SHAPLEY, and when \((m, p) = (100, 30)\), it is even 82 times faster. Furthermore, the results show significant advantages over D-SHAPLEY when \( m \) increases from \( p = 10 \) to \( p = 30 \). The proposed algorithm less depends on \( p \) and even the computational time decreases as \( p \) decreases. This is because we compute a smaller number of expectations due to \( q = p + 10 \). We can efficiently run Algorithm 1 for tens of thousands of data points and thousands of dimensions, and such computation is prohibitive using previous approaches for DShapley. See Supplementary Material.

| Data valuation method | \((m, p)\)       | \((100,10)\) | \((100,30)\) | \((500,10)\) | \((500,30)\) |
|----------------------|-----------------|--------------|--------------|--------------|--------------|
| D-SHAPLEY [14]       | 25.6±1.1        | 115.4±10.5   | 293.0±11.6   | 467.1±11.1   |
| Algorithm 1 (Proposed) | 2.3±0.0        | 1.4±0.0      | 13.0±0.0     | 12.0±0.0     |

### Point removal experiment

We demonstrate the empirical effectiveness of our DShapley approach by running point removal experiments, proposed by Ghorbani and Zou [15]. Given a training dataset to be valued, we recursively remove points from largest to lowest values, retrain the model with the remained dataset, and observe how the utility changes. DShapley does not necessarily ensure a steep performance drop, yet it is expected to decrease fast as removing data points. To empirically verify this, we compare the three methods: (i) the random deletion, (ii) deleting points with the largest Cook’s distance [6], denoted by ‘Cook’, and (iii) deleting points with the largest DShapley estimated using Algorithm 1. We consider three real datasets from the UCI Machine Learning Repository [9] and the Gaussian synthetic datasets used in Figure 1. The real datasets do not satisfy the Gaussian
We can also use the same strategy here and apply Algorithm 1 to the last layer of the network. This would be a straightforward way to extend our results to complex models.

Although the bounds do not perform as good as DShapley in this experiment, they show reasonable performance drops. Note that the upper and lower bounds are computationally very cheap, so the less exact results can be thought as a payoff for the speed-up.

To demonstrate the practical efficacy of the upper and lower bounds in Theorem 3, we conduct another point removal experiment. We compare the four methods: (i) the random deletion, (ii) the lower bound, denoted by ‘Lower’, (iii) the upper bound, denoted by ‘Upper’, and (iv) DShapley based on Algorithm 1. We use the Gaussian synthetic dataset with $m = 500$ and $p = 10$. Figure 3 compares the point removal performance of the four methods. The Spearman’s rank correlation coefficient between ‘Upper’ (resp. ‘Lower’) and DShapley is 0.50 (resp. 0.77). Although the bounds do not perform as good as DShapley in this experiment, they show reasonable performance drops. Note that the upper and lower bounds are computationally very cheap, so the less exact results can be thought as a payoff for the speed-up.

6 Concluding remarks

In this work, we derive analytic expressions for DShapley for the linear regression and non-parametric density estimation problems. The proposed forms provide new mathematical insights, and lead to computationally efficient algorithms. We also demonstrate the efficacy of our results on multiple datasets. One interesting challenge is how to estimate DShapley for more complex nonlinear models such as neural networks. The previous methods for Shapley [15] (and related approaches like influence method) all treat the early layers of the network as fixed feature extractors and apply Shapley to the last layer. This approximates Shapley of the full network, and it achieves good empirical results. We can also use the same strategy here and apply Algorithm 1 to the last layer of the network. This would be a straightforward way to extend our results to complex models.
Broader Impact

Quantification of the value of data has important economic and societal impact. The 2019 Dashboard Act, proposed in the US Senate for example, stipulates that large companies need to quantify the value of the user data that they collect. Such information can then be used to inform regulation, taxation and potentially even compensation. Data Shapley value has been discussed in both ML community and in popular press as a fair approach to data valuation. We are motivated by this to more deeply understand the basic properties of data Shapley value and to propose efficient estimation algorithms. The focus of our work is very much foundational, and it contributes to this topic of growing importance. We recognize that while powerful, Shapley value does not capture many important aspects—e.g. privacy, intrinsic value, etc.—of data. Therefore we emphasize that we are only measuring one component of the value of data.

A Proofs

A.1 Proof of Proposition 1

Proof of Proposition 1 To this end, we fix $S$ and $\gamma$. The ridge estimator based on $S$ and $S \cup \{(x^*, y^*)\}$ are given by

$$\hat{\beta}_{S, \gamma} = A_{S, \gamma}^{-1} X_S^T Y_S,$$

and

$$\hat{\beta}_{S \cup \{(x^*, y^*)\}, \gamma} = (X_{S \cup \{(x^*, y^*)\}}^T X_{S \cup \{(x^*, y^*)\}} + \gamma I_p)^{-1} X_{S \cup \{(x^*, y^*)\}}^T Y_{S \cup \{(x^*, y^*)\}},$$

respectively. By Sherman-Morrison formula,

$$(x^* x^T + A_{S, \gamma})^{-1} = A_{S, \gamma}^{-1} - A_{S, \gamma}^{-1} x^* x^T A_{S, \gamma}^{-1}$$

and

$$\hat{\beta}_{S \cup \{(x^*, y^*)\}, \gamma} = \hat{\beta}_{S, \gamma} + A_{S, \gamma}^{-1} x^* y^* - \frac{A_{S, \gamma}^{-1} x^* x^T \hat{\beta}_{S, \gamma}}{1 + x^T A_{S, \gamma}^{-1} x^*} - \frac{A_{S, \gamma}^{-1} x^* x^T A_{S, \gamma}^{-1} y^*}{1 + x^T A_{S, \gamma}^{-1} x^*},$$

Since $U_{q, \gamma}(S) = (C_{\text{lin}} - \int (y - x^T \hat{\beta}_{S, \gamma})^2 dP_{X,Y}(x, y)) \mathbb{1}(|S| \geq q) = (C_{\text{lin}} - \sigma^2 - (\hat{\beta}_{S, \gamma} - \beta)^T \Sigma_X (\hat{\beta}_{S, \gamma} - \beta)) \mathbb{1}(|S| \geq q)$, for $j - 1 \geq q$, we have

$$\mathbb{E}_{S \sim P_{X,Y}^{k-1}}[U_{q, \gamma}(S \cup \{(x^*, y^*)\})] = C_{\text{lin}} - \sigma^2 - \mathbb{E}_{S \sim P_{X,Y}^{k-1}}[(\hat{\beta}_{S \cup \{(x^*, y^*)\}, \gamma} - \beta)^T \Sigma_X (\hat{\beta}_{S \cup \{(x^*, y^*)\}, \gamma} - \beta)]$$

$$= \mathbb{E}_{S \sim P_{X,Y}^{k-1}}[f_\gamma(X_S)^T \Sigma_X f_\gamma(X_S)] - 2\mathbb{E}_{S \sim P_{X,Y}^{k-1}}[f_\gamma(X_S)^T \Sigma_X (\hat{\beta}_{S, \gamma} - \beta)].$$

Therefore,

$$\mathbb{E}_{S \sim P_{X,Y}^{k-1}}[U_{q, \gamma}(S \cup \{(x^*, y^*)\})] - U_{q, \gamma}(S) = -(\mathbb{E}_{S \sim P_{X,Y}^{k-1}}[f_\gamma(X_S)^T \Sigma_X f_\gamma(X_S)] + 2\mathbb{E}_{S \sim P_{X,Y}^{k-1}}[f_\gamma(X_S)^T \Sigma_X (\hat{\beta}_{S, \gamma} - \beta)],$$

and thus for $q \geq p + 1$, DShapley is

$$\nu((x^*, y^*); U_{q, \gamma}, P_{X,Y}, m) = \frac{1}{m} \sum_{j=1}^{m} \mathbb{E}_{S \sim P_{X,Y}^{k-1}}[U_{q, \gamma}(S \cup \{(x^*, y^*)\})] - U_{q, \gamma}(S)$$
We set
\[ C_{\text{lin}} = \sigma^2 - \mathbb{E}_{S \sim p_X^{-1}}[(\hat{\beta}_{S,\gamma} - \beta)^T \Sigma_X (\hat{\beta}_{S,\gamma} - \beta)] \]
\[ - \frac{1}{m} \sum_{j=1}^{m} \left( \mathbb{E}_{S \sim p_X^{-1}}[f_\gamma(X_j)^T \Sigma_X f_\gamma(X_j)] + 2\mathbb{E}_{S \sim p_X^{-1}}[f_\gamma(X_j)^T \Sigma_X (\hat{\beta}_{S,\gamma} - \beta)] \right). \]

[Step 1] Computation of \( \mathbb{E}[f_\gamma(X_j)^T \Sigma_X f_\gamma(X_j) \mid X_S] \).
We set \( e_{S,\gamma}^* = y^* - x^T \mathbb{E}[\hat{\beta}_{S,\gamma} \mid X_S] = y^* - x^T A_{S,\gamma}^{-1}(X_j^T X_j) \beta, \)
then
\[ \mathbb{E}[f_\gamma(X_j) \mid X_S] = \frac{A_{S,\gamma}^{-1} x^* e_{S,\gamma}^*}{1 + x^T A_{S,\gamma}^{-1} x^*}, \]
and
\[ \text{Cov}[\hat{\beta}_{S,\gamma} \mid X_S] = A_{S,\gamma}^{-1}(X_j^T X_j) A_{S,\gamma}^{-1} \sigma^2 = A_{S,\gamma}^{-1}(A_{S,\gamma} - \gamma I_p) A_{S,\gamma}^{-1} \sigma^2 = A_{S,\gamma}^{-1}(I_p - \gamma A_{S,\gamma}) \sigma^2 = (A_{S,\gamma}^{-1} - \gamma A_{S,\gamma}^{-2}) \sigma^2 =: M_{S,\gamma} \sigma^2 \]
gives
\[ \text{Cov}[f_\gamma(X_j) \mid X_S] = \frac{A_{S,\gamma}^{-1} x^* x^T M_{S,\gamma} x^* x^T A_{S,\gamma}^{-1}}{(1 + x^T A_{S,\gamma}^{-1} x^*)^2} \sigma^2. \]
Thus,
\[ \mathbb{E}[f_\gamma(X_j)^T \Sigma_X f_\gamma(X_j) \mid X_S] = \frac{x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} x^*}{(1 + x^T A_{S,\gamma}^{-1} x^*)^2} e_{S,\gamma}^* + \frac{x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} x^*}{(1 + x^T A_{S,\gamma}^{-1} x^*)^2} x^T M_{S,\gamma} x^* \sigma^2. \]
Since
\[ e_{S,\gamma}^* = e^* + x^T (\beta - A_{S,\gamma}^{-1}(X_j^T X_j) \beta) = e^* + x^T A_{S,\gamma}^{-1} \beta, \]
and \( M_{S,\gamma} = A_{S,\gamma}^{-1} - \gamma A_{S,\gamma}^{-2} \), we have
\[ \mathbb{E}[f_\gamma(X_j)^T \Sigma_X f_\gamma(X_j) \mid X_S] = \frac{x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} x^*}{(1 + x^T A_{S,\gamma}^{-1} x^*)^2} \left( \left( e^* + x^T A_{S,\gamma}^{-1} \right)^2 \sigma^2 + x^T A_{S,\gamma}^{-1} x^* \right) + h_1(\gamma), \]
where \( h_1(\gamma) \) is some explicit term such that \( \lim_{\gamma \to 0^+} h_1(\gamma)/(\gamma \log(\gamma)) = 0 \).

[Step 2] Computation of \( \mathbb{E}[f_\gamma(X_j)^T \Sigma_X (\hat{\beta}_{S,\gamma} - \beta) \mid X_S] \).

\[ \mathbb{E}[f_\gamma(X_j)^T \Sigma_X (\hat{\beta}_{S,\gamma} - \beta) \mid X_S] = \mathbb{E}\left[ \left( y^* - x^T \hat{\beta}_{S,\gamma} \right)^T x^T A_{S,\gamma}^{-1} \Sigma_X (\hat{\beta}_{S,\gamma} - \beta) \right] \mid X_S \]
\[ = -\frac{e^* x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} \beta}{1 + x^T A_{S,\gamma}^{-1} x^*} - \mathbb{E}_S[\hat{\beta}_{S,\gamma}^T (\hat{\beta}_{S,\gamma} - \beta)^T x^* x^T A_{S,\gamma}^{-1} \Sigma_X (\hat{\beta}_{S,\gamma} - \beta) \mid X_S] \]
\[ = -\frac{e^* x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} \beta}{1 + x^T A_{S,\gamma}^{-1} x^*} - \frac{e^* x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} \beta}{1 + x^T A_{S,\gamma}^{-1} x^*} - \frac{2\beta A_{S,\gamma}^{-1} x^* x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} \beta}{1 + x^T A_{S,\gamma}^{-1} x^*} - \frac{x^T A_{S,\gamma}^{-1} \Sigma_X M_{S,\gamma} x^*}{1 + x^T A_{S,\gamma}^{-1} x^*} \sigma^2 \]
\[ = -\frac{x^T A_{S,\gamma}^{-1} \Sigma_X A_{S,\gamma}^{-1} x^*}{1 + x^T A_{S,\gamma}^{-1} x^*} \sigma^2 + h_2(\gamma). \]

where \( h_2(\gamma) \) is some explicit term such that \( \lim_{\gamma \to 0^+} h_2(\gamma)/(\gamma \log(\gamma)) = 0 \) and \( h_2(0) = 0 \).

Hence, by setting \( C_{\text{lin}} = \sigma^2 + \mathbb{E}_{S \sim p_X^{-1}}[(\hat{\beta}_{S,\gamma} - \beta)^T \Sigma_X (\hat{\beta}_{S,\gamma} - \beta)] \), we have
\[ \nu((x^*, y^*); U_{q, \gamma}, P_{X,Y}, m) = C_{\text{lin}} - \sigma^2 - \mathbb{E}_{S \sim p_X^{-1}}[(\hat{\beta}_{S,\gamma} - \beta)^T \Sigma_X (\hat{\beta}_{S,\gamma} - \beta)] \]
- \frac{1}{m} \sum_{j=1}^{m} E_{X_{S} \sim P_{X}^{\gamma^{-1}}} \left[ x^{T} A_{S,\gamma}^{-1} \Sigma_{X} A_{S,\gamma}^{-1} x \right] + h(\gamma), \quad (6)

= - \frac{1}{m} \sum_{j=1}^{m} E_{X_{S} \sim P_{X}^{\gamma^{-1}}} \left[ x^{T} A_{S,\gamma}^{-1} \Sigma_{X} A_{S,\gamma}^{-1} x \right] + h(\gamma),

= \frac{1}{m} \sum_{j=1}^{m} E_{X_{S} \sim P_{X}^{\gamma^{-1}}} \left[ x^{T} A_{S,\gamma}^{-1} \Sigma_{X} A_{S,\gamma}^{-1} x \right] + h(\gamma),

for some \( h(\gamma) \) such that \( \lim_{\gamma \to 0^+} h(\gamma)/\gamma \log(\gamma) = 0 \) and \( h(0) = 0 \).

A.2 Proof of Theorem 2

Proof of Theorem 2

By plugging \( \gamma = 0 \) into Equation (6), for \( q \geq p + 3 \), DShapley is given by

\[
\nu((x^*, y^*); U_{q,0}, P_{X,Y}, m) = C_{lin} - \sigma^2 - E_{X \sim P_X^{-1}}[(\tilde{\beta}_{S,\gamma} - \beta)^T \Sigma_{X} (\tilde{\beta}_{S,\gamma} - \beta)] + \frac{\sigma^2}{m} \sum_{j=1}^{m} \left( 1 - \frac{e^{x_j^T x_j}}{\sigma^2} \right) E_{X_{S} \sim P_{X}^{\gamma^{-1}}} \frac{x_j^{T} (X_j^T \tilde{X}_S)^{-2} x_j}{(1 + x_j^{T} (X_j^T \tilde{X}_S)^{-1} x_j)^2} + E_{X_{S} \sim P_{X}^{\gamma^{-1}}} \left[ \frac{x_j^{T} (X_j^T \tilde{X}_S)^{-2} x_j}{(1 + x_j^{T} (X_j^T \tilde{X}_S)^{-1} x_j)^2} \right],
\]

(7)

where \( \tilde{X}_S = X_S \Sigma_X^{-1/2} \) and \( \tilde{x}^* = \Sigma_X^{-1/2} x^* \), i.e., a normalized version. Note that \( (\tilde{X}_S^T \tilde{X}_S)^{-1} \) follows an inverse-Wishart distribution and its mean is \( I_p/(q-1-p-1) \). Therefore,

\[
- \frac{\sigma^2}{m} \text{tr} \left( E_{X_{S} \sim P_{X}^{\gamma^{-1}}} [(\tilde{X}_S^T \tilde{X}_S)^{-1}] \right) = \frac{\sigma^2}{m} \frac{p}{q-p-2}.
\]

Now it is enough to compute the following expectations:

\[
E_{X_{S} \sim P_{X}^{\gamma^{-1}}} \left[ \frac{x_j^{T} (X_j^T \tilde{X}_S)^{-2} x_j}{(1 + x_j^{T} (X_j^T \tilde{X}_S)^{-1} x_j)^2} \right] \quad \text{and} \quad E_{X_{S} \sim P_{X}^{\gamma^{-1}}} \left[ \frac{x_j^{T} (X_j^T \tilde{X}_S)^{-2} x_j}{(1 + x_j^{T} (X_j^T \tilde{X}_S)^{-1} x_j)^2} \right].
\]

[Step 1] For any \( p \times p \) orthogonal matrix \( \Gamma \), we have \( \Gamma (\tilde{X}_S^T \tilde{X}_S) \Gamma^T \sim W_p(|S|, I_p) \) due to \( \tilde{X}_S^T \tilde{X}_S \sim W_p(|S|, I_p) \). We choose an orthogonal matrix \( \Gamma \) with the first column is \( (\tilde{x}^T \tilde{x}^*)^{-1/2} \tilde{x}^* \) and let \( V \coloneqq \Gamma (\tilde{X}_S^T \tilde{X}_S) \Gamma^T \). Then, \( \tilde{x}^T (\tilde{X}_S^T \tilde{X}_S)^{-1} \tilde{x}^* = (\Gamma \tilde{x}^*)^T V^{-1} (\Gamma \tilde{x}^*) = \tilde{x}^T \tilde{x}^* v^{11} \) where \( V^{-1} = (v^{ij}) \). Similarly, we obtain \( \tilde{x}^T (\tilde{X}_S^T \tilde{X}_S)^{-1} \tilde{x}^* = \tilde{x}^T \tilde{x}^* \sum_{j=1}^{p} (v^{1j})^2 \).

Now we let \( V = TT^T \) where \( T \) is an upper triangular matrix with positive diagonal elements as

\[
T = \begin{pmatrix} t_{11}^{-1} & t^T \\ 0 & T_{22}^{-1} \end{pmatrix}.
\]

Then,

\[
T^{-1} = \begin{pmatrix} t_{11}^{-1} & -t_{11}^{-1} t T_{22}^{-1} \\ 0 & T_{22}^{-1} \end{pmatrix}, \quad V^{-1} = \begin{pmatrix} t_{11}^{-2} & -t_{11}^{-2} t T_{22}^{-1} \\ -t_{11}^{-2} t T_{22}^{-1} & (T_{22}^T T_{22})^{-1} + t_{11}^{-2} (T_{22}^T T_{22})^{-1} tt^T T_{22}^{-1} \end{pmatrix}.
\]

Therefore,

\[
\frac{\tilde{x}^T (\tilde{X}_S^T \tilde{X}_S)^{-2} \tilde{x}^*}{(1 + \tilde{x}^T (\tilde{X}_S^T \tilde{X}_S)^{-1} \tilde{x}^*)^2} = \frac{\tilde{x}^T \tilde{x}^* (t_{11}^{-4} + t_{11}^{-4} t T_{22}^T T_{22}^{-1} t)}{(1 + \tilde{x}^T t T_{22}^{-1} t)^2} = \frac{\tilde{x}^T \tilde{x}^* (1 + t T_{22} T_{22}^{-1} t)}{(\tilde{x}^T \tilde{x}^* + t_{11}^{-1})^2}.
\]

Thanks to Gupta and Nagar [19, Theorem 3.3.5], \( t_{11}^2 \) is independent to \( t^T (T_{22}^T T_{22})^{-1} t \) with \( t_{11}^2 \sim \chi_{|S|-p+1}^2 \). Furthermore, by Gupta and Nagar [19, Theorem 3.3.28], \( t^T (T_{22}^T T_{22})^{-1} t \sim \chi_{|S|-p+1} \).

That is,

\[
E_{X \sim P_X^{-1}} \left[ \frac{\tilde{x}^T (\tilde{X}_S^T \tilde{X}_S)^{-2} \tilde{x}^*}{(1 + \tilde{x}^T (\tilde{X}_S^T \tilde{X}_S)^{-1} \tilde{x}^*)^2} \right] = \tilde{x}^T \tilde{x}^* E[(1 + t T_{22} T_{22}^{-1} t)] E\left[ \frac{1}{(\tilde{x}^T \tilde{x}^* + t_{11}^{-1})^2} \right].
\]
we have \( \| X \|_{\psi_2} := \sup \| x \|_{1} \| X \|_{\psi_2} \). Lastly, we quote the non-asymptotic eigenvalue bounds by Vershynin [32] Theorem 5.39.

**Lemma 5.** Suppose that \( \tilde{X}_S \) is a matrix whose rows are independent sub-Gaussian isotropic random vectors in \( \mathbb{R}^p \), then for every \( t \geq 0 \), with probability at least \( 1 - 2 \exp(-ct^2) \) one has

\[
\sqrt{|S|}(1 - \delta_{|S|}) = \sqrt{|S|} - C\sqrt{|p|} - t \leq \lambda_{\min}(\tilde{X}_S) \leq \lambda_{\max}(\tilde{X}_S) \leq \sqrt{|S|} + C\sqrt{|p|} + t = \sqrt{|S|}(1 + \delta_{|S|}),
\]

where \( \delta_{|S|} = (C\sqrt{|p|} + t)/\sqrt{|S|} \) and \( C, c \) are two constants depending only on the sub-Gaussian norm.
Proof of Theorem 3 [Step 1] We provide a proof for the upper bound only, but the similar procedure can show the lower bound. To this end, we fix \( S \) and let \( \tilde{X}_S = X_S \Sigma_X^{-1/2}, \tilde{x}^* = \Sigma_X^{1/2} x^* \), and \( \tilde{A}_y = (\tilde{X}_S^T \tilde{X}_S + \gamma \Sigma_X^{-1}) \). Then, we have

\[
\frac{x^* A_y^{-1} x^2}{1 + x^* A_y^{-1} x^2} \leq \frac{(\tilde{x}^* \tilde{A}_y^{-2} \tilde{x}^*) (2 + \tilde{x}^* \tilde{A}_y^{-1} \tilde{x}^*) \sigma^2 + e^2}{(1 + \tilde{x}^* \tilde{A}_y^{-1} \tilde{x}^*)^2}.
\]

(8)

Due to \( \lambda_{\text{max}}(AB) \leq \lambda_{\text{max}}(A) \lambda_{\text{max}}(B) \), we have

\[
\frac{(\tilde{x}^* \tilde{A}_y^{-2} \tilde{x}^*) (2 + \tilde{x}^* \tilde{A}_y^{-1} \tilde{x}^*) \sigma^2 + e^2}{(1 + \tilde{x}^* \tilde{A}_y^{-1} \tilde{x}^*)^2} \leq \frac{\tilde{x}^* \tilde{x}^* \lambda_{\text{max}}(\tilde{A}_y^{-2}) (2 + \tilde{x}^* \tilde{x}^* \lambda_{\text{max}}(\tilde{A}_y^{-1}))}{(1 + \tilde{x}^* \tilde{x}^* \lambda_{\text{min}}(\tilde{A}_y^{-1}))^2} \sigma^2 + \frac{1}{(1 + \tilde{x}^* \tilde{x}^* \lambda_{\text{max}}(\tilde{A}_y^{-1}))^2} e^2.
\]

Since \( |y_i| \leq B \) and \( \beta_{R,S}^\theta = \arg\min_\beta (Y_S - X_S \beta)^T (Y_S - X_S \beta) + \gamma \|\beta\|_2^2 \), we obtain boundedness of \( \|\beta_{R,S}^\theta\|_2 \), i.e., \( \|\beta_{R,S}^\theta\|_2 \leq \gamma \|Y_S - X_S \beta\|_2 \leq \gamma^{-1} m B_S^2 \) for any \( S \subseteq \mathcal{X} \). That means, \( U_{S}^R(S) \) is bounded, and thus Equation (8) is bounded as well. Let say the bound is \( C_{\text{bdd}} \).

[Step 2] Using Lemma 3 with \( t_{|S|} = \sqrt{\frac{\log(|S|m^{1/2})}{e}} \), the following holds with probability at least \( 1 - 2/(|S|m^{1/2}) \).

\[
\sqrt{|S|} (1 - \delta_{|S|}) = \sqrt{|S|} - C \sqrt{p} - t \leq \lambda_{\text{min}}(\tilde{X}_S) \leq \lambda_{\text{max}}(\tilde{X}_S) \leq \sqrt{|S|} + C \sqrt{p} + t = \sqrt{|S|} (1 + \delta_{|S|}),
\]

where \( \delta_{|S|} = (C \sqrt{p} + \sqrt{\frac{\log(|S|m^{1/2})}{2e}}) / \sqrt{|S|} \). We denote the set where the inequalities hold by \( \Omega_{|S|} \) and we obtain the following bounds.

\[
\begin{align*}
&\mathbb{E}_{X_S \sim P_X^{-1}} \left[ (\tilde{x}^* \tilde{A}_y^{-2} \tilde{x}^*) (2 + \tilde{x}^* \tilde{A}_y^{-1} \tilde{x}^*) \sigma^2 + e^2) \right] \\
&\leq \int_{\Omega_{|S|}} \frac{\tilde{x}^* \tilde{x}^* \lambda_{\text{max}}(\tilde{A}_y^{-2}) (2 + \tilde{x}^* \tilde{x}^* \lambda_{\text{max}}(\tilde{A}_y^{-1}))}{(1 + \tilde{x}^* \tilde{x}^* \lambda_{\text{min}}(\tilde{A}_y^{-1}))^2} \sigma^2 dP - \int_{\Omega_{|S|}} \frac{1}{(1 + \tilde{x}^* \tilde{x}^* \lambda_{\text{max}}(\tilde{A}_y^{-1}))^2} e^2 dP + C_{\text{bdd}} dP
\end{align*}
\]

where the second inequality is due to \( \lambda_{\text{min}}(A + B) \geq \lambda_{\text{min}}(A) + \lambda_{\text{min}}(B) \) and \( \lambda_{\text{max}}(A + B) \leq \lambda_{\text{max}}(A) + \lambda_{\text{max}}(B) \). Hence,

\[
\nu((x^*, y^*); U_{q, \gamma}, P_{X, Y, m})
\]

\[
\begin{align*}
&\leq \frac{1}{m} \sum_{j=q-1}^{m-1} \frac{x^*^T x^* (j(1 - \delta_j)^2 + \gamma \lambda_{\text{min}}(\Sigma_X^{-1}))^{-1/2}}{(1 + x^*^T x^*(j(1 + \delta_j)^2 + \gamma \lambda_{\text{max}}(\Sigma_X^{-1}))^{-1/2})^2} \left( 2 + \tilde{x}^* \tilde{x}^* (j(1 - \delta_j)^2 + \gamma \lambda_{\text{min}}(\Sigma_X^{-1}))^{-1/2} \sigma^2 \\
&- \frac{1}{m} \sum_{j=q-1}^{m-1} \frac{e^2}{(1 + x^*^T x^*(j(1 - \delta_j)^2 + \gamma \lambda_{\text{min}}(\Sigma_X^{-1}))^{-1/2})^2} + \frac{C_{\text{bdd}}}{m} \sum_{j=q-1}^{m-1} P(\Omega_j^c) + h(\gamma)
\end{align*}
\]

\[
= \frac{1}{m} \sum_{j=q-1}^{m-1} \frac{x^*^T x^* A_{\text{upper}}(j)}{(1 + x^*^T x^* A_{\text{lower}}(j))^2} \left( 2 + \tilde{x}^* \tilde{x}^* A_{\text{upper}}(j) \right) \sigma^2 \\
&- \frac{1}{m} \sum_{j=q-1}^{m-1} \frac{e^2}{(1 + x^*^T x^* A_{\text{upper}}(j))^2} + \frac{C_{\text{bdd}}}{m} \sum_{j=q-1}^{m-1} P(\Omega_j^c) + h(\gamma),
\]

13
where $\Lambda_{\text{upper}}(j) := (j(1 - \delta_j)^2 + \gamma \lambda_{\text{min}}(\Sigma_X^{-1}))^{-1}$ and $\Lambda_{\text{lower}}(j) := (j(1 + \delta_j)^2 + \gamma \lambda_{\text{max}}(\Sigma_X^{-1}))^{-1}$ for $j \in \mathbb{N}$. Lastly, $\frac{1}{m} \sum_{j=q-1}^{m-1} P(\Omega_j) = \frac{1}{m} \sum_{j=q-1}^{m-1} \frac{2}{j \sqrt{m}} \leq 4 \log(m) / m^{3/2}$ concludes a proof. \[\square\]

**Remark 1.** It is noteworthy that the eigenvalues of $A_{S,\gamma}^{-1}$ are contained in $[\Lambda_{\text{lower}}(j), \Lambda_{\text{upper}}(j)]$ with high probability. By Lemma 5 on $\Omega_j$, we have

$$j(1 - \delta_j)^2 + \gamma \lambda_{\text{min}}(\Sigma_X^{-1}) \leq \lambda_{\text{min}}(A_{S,\gamma}) \leq \lambda_{\text{max}}(A_{S,\gamma}) \leq j(1 + \delta_j)^2 + \gamma \lambda_{\text{max}}(\Sigma_X^{-1}),$$

and thus

$$\Lambda_{\text{lower}}(j) \leq \lambda_{\text{min}}(A_{S,\gamma}^{-1}) \leq \lambda_{\text{max}}(A_{S,\gamma}^{-1}) \leq \Lambda_{\text{upper}}(j).$$

### A.4 Proof of Theorem 4

**Proof of Theorem 4** Let $S^* = \{z_1^*, \ldots, z_n^*\}$. A simple algebra gives $\hat{p}_{S \cup S^*}(z) = \frac{1}{|S| + n} (\sum_{j=1}^n k(z, z_j^*) + |S| \hat{p}_S(z)) = \frac{1}{|S| + n} \sum_{j=1}^n k(z, z_j^*) + \frac{|S|}{|S| + n} \hat{p}_S(z) = \hat{p}_S(z) + \frac{n}{|S| + n} \sum_{j=1}^n k(z, z_j^*) - \hat{p}_S(z)$. Note that $\frac{1}{n} \sum_{j=1}^n k(z, z_j^*) = \hat{p}_S(z)$. For $|S| \geq 1$, we have

$$U(S \cup S^*) - U(S) = - \int (p(z) - \hat{p}_{S \cup S^*}(z))^2 - (p(z) - \hat{p}_S(z))^2 dz$$

$$= - \int \left( \frac{n}{|S| + n} (\hat{p}_S(z) - \hat{p}_S(z))^2 - (p(z) - \hat{p}_S(z)\right)^2 dz$$

$$= - \int \frac{n^2}{(|S| + n)^2} (\hat{p}_S(z) - \hat{p}_S(z))^2 - \frac{2n}{|S| + n} \left\{ (p(z) - \hat{p}_S(z))(\hat{p}_S(z) - \hat{p}_S(z)) \right\} dz.$$

Furthermore,

$$\left(\hat{p}_S(z) - \hat{p}_S(z)\right)^2 = (\hat{p}_S(z) - p(z) + p(z) - \hat{p}_S(z))^2$$

$$= (\hat{p}_S(z) - p(z))^2 + (p(z) - \hat{p}_S(z))^2 + 2(\hat{p}_S(z) - p(z))(p(z) - \hat{p}_S(z)),$$

and

$$\left(\hat{p}_S(z) - \hat{p}_S(z)\right)(\hat{p}_S(z) - \hat{p}_S(z)) = (p(z) - \hat{p}_S(z))(\hat{p}_S(z) - p(z) + p(z) - \hat{p}_S(z))$$

$$= (p(z) - \hat{p}_S(z))(\hat{p}_S(z) - p(z)) + (p(z) - \hat{p}_S(z))^2.$$

Equations (9) and (10) give

$$\mathbb{E}[U(S \cup S^*) - U(S)] = - \frac{n^2}{(|S| + n)^2} \int (\hat{p}_S(z) - p(z))^2 dz$$

$$+ \frac{n^2 + 2n|S|}{(|S| + n)^2} \int \mathbb{E}[(p(z) - \hat{p}_S(z))^2] dz$$

$$+ \frac{n|S|}{(|S| + n)^2} \int (\hat{p}_S(z) - p(z))\mathbb{E}[p(z) - \hat{p}_S(z)] dz.$$

We can decompose $\mathbb{E}[U(S \cup S^*) - U(S)]$ into two terms by dependency of $S^*$. To be more specific,

$\mathbb{E}[U(S \cup S^*) - U(S)] = h_1(S^*, |S|) + h_2(|S^|, |S|)$

where

$$h_1(S^*, |S|) = - \frac{n^2}{(|S| + n)^2} \int (\hat{p}_S(z) - p(z))^2 dz + \frac{2n|S|}{(|S| + n)^2} \int \hat{p}_S(z)\mathbb{E}[p(z) - \hat{p}_S(z)] dz.$$

Also,

$$h_2(n, |S|) = \frac{n^2 + 2n|S|}{(|S| + n)^2} \int \mathbb{E}[(p(z) - \hat{p}_S(z))^2] dz - \frac{2n|S|}{(|S| + n)^2} \int p(z)\mathbb{E}[p(z) - \hat{p}_S(z)] dz$$

$$= \frac{n^2 + 2n|S|}{(|S| + n)^2} \int \mathbb{E}[(p(z) - \hat{p}_S(z))^2] dz - \frac{2n|S|}{(|S| + n)^2} \int p(z)(p(z) - \mathbb{E}[k(z, Z)]) dz.$$
Therefore, by Ghorbani et al. [14, Theorem 2.3], we have

\[
\nu(S^*, U, P, m) = \frac{1}{m} \sum_{j=1}^{m} \mathbb{E}_{S \sim P_{j-1}} [U(S \cup S^*) - U(S)]
\]

\[
= -\frac{1}{m} \sum_{j=1}^{m} \sum_{k=1}^{n^2} \left( \frac{n^2}{(j+n-1)^2} \int (\hat{p}_{S^*}(z) - p(z))^2 dz \right)
\]

\[
+ \frac{1}{m} \sum_{j=2}^{m} 2n(j-1) \left( \frac{2n(j-1)}{(j+n-1)^2} \int \hat{p}_{S^*}(z)(p(z) - \mathbb{E}[k(z, Z)])dz + C_0(n, m) \right)
\]

\[
= -A(n, m) \int (\hat{p}_{S^*}(z) - p(z))^2 dz + B(n, m)g(S^*) + C_0(n, m), \quad (11)
\]

and

\[
C_0(n, m) = \frac{1}{m} C_{\text{den}} + \frac{1}{m} \sum_{j=2}^{m} h_2(n, j - 1). \quad (12)
\]

Hence, it concludes a proof by choosing the constant \( C_{\text{den}} \) as follows.

\[
C_{\text{den}} = -\sum_{j=2}^{m} h_2(n, j - 1).
\]
B Details for Examples in Section 4

B.1 Details for Example 1

Proof of Example 1 A key idea is to develop Equation (11).

[Step 1] In this step we compute

\[ h_2(n, |S|) = \frac{n^2 + 2n|S|}{(|S| + n)^2} \int \mathbb{E}[(p(z) - \hat{p}_S(z))^2]dz - \frac{2n|S|}{(|S| + n)^2} \int p(z)(p(z) - \mathbb{E}[k(z, Z)])dz. \]

We first compute the term \( \int \mathbb{E}[(p(z) - \hat{p}_S(z))^2]dz \). Note that \( \hat{p}_S^2(z) = \frac{1}{|S|^2}(\sum_{i \in S} k(z, z_i) + \sum_{i \neq j} k(z, z_i)k(z, z_j)) \). We have

\[
\mathbb{E}[:p_S(z)] = \mathbb{E}[k(z, Z)] = \begin{cases} 
\frac{1}{2} + \frac{z}{h}, & 0 \leq z \leq h/2, \\
1, & h/2 \leq z \leq 1 - h/2, \\
\frac{1}{2} + \frac{1-z}{h}, & 1 - h/2 \leq z \leq 1,
\end{cases}
\]

and due to \( p(z) = 1 \),

\[ p(z) - \mathbb{E}[k(z, Z)] = \begin{cases} 
\frac{1}{2} - \frac{z}{h}, & 0 \leq z \leq h/2, \\
0, & h/2 \leq z \leq 1 - h/2, \\
\frac{1}{2} - \frac{1-z}{h}, & 1 - h/2 \leq z \leq 1.
\end{cases} \]

Since \( S \) are randomly sampled, we have

\[ \mathbb{E}[:p_S^2(z)] = \frac{|S|\mathbb{E}[k(z, Z)]/h + |S|(|S| - 1)\mathbb{E}[k(z, Z)]^2}{|S|^2} = \frac{\mathbb{E}[k(z, Z)]}{|S|h} + \frac{|S| - 1}{|S|}\mathbb{E}[k(z, Z)]^2. \]

Furthermore, we have \( \int \mathbb{E}[k(z, Z)]dz = 1 - h/4 \) and \( \int \mathbb{E}[k(z, Z)]^2dz = 1 - 5h/12 \). Hence,

\[ \int \mathbb{E}[(p(z) - \hat{p}_S(z))^2]dz = 1 + \left( \mathbb{E}[k(z, Z)] - \frac{|S| - 1}{|S|}(1 - \frac{5h}{12}) \right) - 2 \left( 1 - \frac{h}{4} \right) = \frac{1}{|S|h} + \frac{5 - 4|S|}{12|S|}h \]

Lastly, \( \int p(z)(p(z) - \mathbb{E}[k(z, Z)])dz = h/4 \) gives

\[ h_2(n, |S|) = \frac{n^2 + 2n|S|}{(|S| + n)^2} \frac{12 - 15h + (5 + |S|)h^2}{12|S|h} - \frac{2n|S|}{(|S| + n)^2} \frac{h}{4}. \]

[Step 2] By construction of \( h \), \( g(S^*) = 0 \). If \( \Delta \geq h \), since \( z_1^* \) and \( z_2^* \) are apart at least \( h \),

\[ -\int (p(z) - \hat{p}_{S^*}(z))^2dz = -\int (1 - \hat{p}_{S^*}(z))^2dz = \left( |S^*|h \left( 1 - \frac{1}{|S^*|h} \right)^2 + (1 - |S^*|h) \right) = 1 - \frac{1}{|S^*|h}. \]

Therefore, by aggregating all the results in [Step 1] and [Step 2], we have

\[ \nu(S^*; U, P, m) = A(2, m) \left( 1 - \frac{1}{2h} \right) + C_0(2, m). \]
Note that by Equation (12),
\[ C_0(2, m) = \frac{1}{m} C_{\text{den}} + \frac{1}{m} \sum_{j=2}^{m} h_2(2, j - 1). \]

Note that we set \( C_{\text{set}} = C_0(2, m) \) in the manuscript.

[Step 3] We now consider the case \( \Delta < h \). To this end, without loss of generality, we assume that \( z_1^* \leq z_2^* \). Then there is overlap between \((z_1^* - h/2, z_1^* + h/2)\) and \((z_2^* - h/2, z_2^* + h/2)\).

\[ \hat{p}_{S^*}(z) = \begin{cases} \frac{1}{2h} & z_1^* - h/2 \leq z \leq z_2^* - h/2, \\ \frac{1}{h} & z_2^* - h/2 \leq z \leq z_1^* + h/2, \\ \frac{1}{2h} & z_1^* + h/2 \leq z \leq z_2^* + h/2, \\ 0 & \text{otherwise}. \end{cases} \]

Therefore, \( \int (p(z) - \hat{p}_{S^*}(z))^2 dz = -1 + \frac{1}{h} - \frac{\Delta}{2h^2} \). Hence, we have
\[ \nu(S^*; U, P, m) = A(2, m) \left( 1 - \frac{1}{h} + \frac{\Delta}{2h^2} \right) + C_0(2, m). \]

\( \Box \)

B.2 Details for Example 2

A similar analysis used in Example 1 gives
\[ \nu(z_1^*; U, P_Z, m) = A(1, m)(1 - \frac{1}{h}) + C_0(1, m), \]
where \( C_0(1, m) = \frac{1}{m} C_{\text{den}} + \frac{1}{m} \sum_{j=2}^{m} h_2(1, j - 1) \) by Equation (12). Since it is difficult to solve (5) analytically, we numerically examine when (5) holds when \( C_{\text{den}} = 0.2 \) and \( m = 100 \). For fixed bandwidth \( h \), we randomly draw \( S^* \) 5000 times and observe if there is a synergy. We empirically recognize that the synergy is determined by \( \Delta \) so we define the synergy threshold as the smallest \( \Delta \) when the synergy happens, i.e., if \( \Delta \) is greater than the synergy threshold, the inequality
\[ \nu(z_1^*; U, P_Z, m) \geq \nu(z_1^*; U, P_Z, m) + \nu(z_2^*; U, P_Z, m) \]
holds. Also, among the 5000 random sampled sets \( S^* \), we estimate probability that the synergy happens. Figure 4 shows that the synergy threshold and the corresponding synergy probability as a function of \( h \). As \( h \) increases, the synergy threshold (in red dotted) increases and the synergy probability (in blue solid) decreases, meaning that in all bandwidths \( h \in (0, 0.35) \), the synergy happens when the two points in \( S^* \) is far apart to some extent.

Figure 4: The synergy threshold (red dotted) and the corresponding synergy probability (blue solid) as a function of bandwidth.
C Implementation details

In this section, we provide implementation details including comprehensive information for Algorithm 1, datasets, and experiment settings.

Algorithm We present a detailed version of Algorithm 1. We use $\rho_1 = 0.01$ and $\rho_2 = 0.005$ for all experiments.

Algorithm 2 A distributional Shapley value for the least square estimator under Gaussian inputs

Require: True value or estimates for $x^*\Sigma_x^{-1}x^*, e^2$, and $\sigma^2$. Thresholds $\rho_1, \rho_2$. The maximum number of Monte Carlo samples $T$. A constant $q \geq p + 3$.

procedure
  Initialize $\hat{\nu}^{\text{old}} \leftarrow 0$
  for $j \in \{q, \ldots, m\}$ do
    Initialize $A_j^{\text{old}} \leftarrow 0$
    for $i \in \{1, \ldots, T\}$ do
      Sample $t_{[i]}$ from the $\chi^2_{j-p+1}$.
      $A_j^{\text{new}} \leftarrow (i - 1)A_j^{\text{old}} + \frac{i - 1}{j-p} x^*\Sigma_x^{-1}x^*e^2 + t_{[i]}\sigma^2$ \quad $\triangleright$ Based on Theorem 2
      if $|A_j^{\text{new}}/A_j^{\text{old}} - 1| \leq \rho_1$ then
        break
      end if
    end for
    $\hat{\nu}^{\text{old}} \leftarrow A_j^{\text{old}}$
  end for
  $\hat{\nu}^{\text{new}} \leftarrow \hat{\nu}^{\text{old}} - \frac{A_j^{\text{new}}}{m}$
  if $|\hat{\nu}^{\text{old}}/\hat{\nu}^{\text{new}} - 1| \leq \rho_2$ then
    break
  end if
  $\hat{\nu}^{\text{old}} \leftarrow \hat{\nu}^{\text{new}}$
end procedure \quad $\triangleright$ Estimates for DShapley

Datasets As for the Gaussian synthetic datasets, given $(m, p)$ and $\beta$, we generate $y_i = x_i^T \beta + \epsilon_i$ for all $i \in [m]$, where $x_i \sim \mathcal{N}(0, I_p)$ and $\epsilon_i \sim \mathcal{N}(0, 1)$. As for the real datasets, we use the six real datasets from the UCI Machine Learning Repository [9] and Efron et al. [12]. A summary of basic statistics is provided in Table 2. Among them, we use abalone, redwine, and whitewine in the manuscript. The other three datasets are used in Appendix.

Table 2: A summary of the three regression datasets.

| Dataset  | # of samples | $d$ | Source          |
|----------|--------------|-----|-----------------|
| abalone  | 4177         | 10  | UCI Repository  |
| airfoil  | 1503         | 5   | UCI Repository  |
| boston   | 506          | 13  | UCI Repository  |
| diabetes | 442          | 10  | Efron et al. [12] |
| redwine  | 1599         | 11  | UCI Repository  |
| whitewine| 4898         | 11  | UCI Repository  |

Time comparison experiment We use the Gaussian synthetic datasets with various $(m, p)$ and measure the elapsed time for running an algorithm for the whole dataset, i.e., the elapsed time for $m$ data points.

Point removal experiment The point removal experiment consists of the two steps: (i) given a dataset to be valued, we first estimate the values, and (ii) based on values, we remove data from largest to lowest value, compute a predefined utility function. Note that we use additional data points to estimate the utility function in the second step. As for the Gaussian synthetic datasets, we assume that the underlying distribution is known. We generate additional 2000 data points from the true distribution and estimate the utility. Since we do not know the underlying distribution of the real
datasets, so as for the real datasets, we split randomly the original dataset into the two datasets with 80% and 20%. We regard the 80% data points as a set to be valued and we use another 20% data points for the utility evaluation.

In all experiments, the constant $C_{\text{lin}} = 2\hat{\sigma}^2$, where $\hat{\sigma} := \frac{1}{m-p} \sum_{i=1}^{m-p} (y_i - x_i^T \hat{\beta})^2$ and $\hat{\beta}$ is the least square estimator based on the full dataset\footnote{Here, we simply reset the index for notational convenience.}. In Figures 2 and 3 we use the relative utility defined as $100 \times \frac{U(S_i)}{U(B)}$ where $S_i$ is a remaining subset of $B$ at $i$-th removal time. Lastly, as for Figure 3, we use the upper and lower bounds based on Theorem 3. We fix the hyperparameters $\gamma = 1/m$, $q = p + 20$, $C = 0.1$, and $c = 0.5$ in Lemma 5 and compute the upper and lower bounds by computing $\Lambda_{\text{upper}}$ and $\Lambda_{\text{lower}}$. In all experiments, the number of repetitions is 10.
D Additional numerical experiments

D.1 Additional results for Figure 1

Here, we illustrate DShapley when $p = 30$ as Figure 1. We use the same Gaussian synthetic dataset, but the input dimension is $p = 30$. Overall it shows similar results to when $p = 10$.

![Figure 5: The illustration of DShapley as a function of the Mahalanobis distance $x^T \Sigma_x^{-1} x$ when $p = 30$. Different colors indicate different error levels.](image)

D.2 Additional results for the computational time

We consider various large $(m, p)$ settings and measure the computational time. We observe that for one repetition $D$-SHAPLEY by Ghorbani et al. [14] exceeds more than seven hours (resp. two days) when $(m, p) = (1000, 500)$ (resp. when $(m, p) = (2000, 1000)$). It is not feasible to repeat 10 times for larger $(m, p)$, so we report the results for the proposed method only. As shown in Table 3, the proposed method runs in reasonable times and clearly shows its efficiency.

Table 3: A summary of the computational time (in seconds) of Algorithm 1 in various $(m, p)$. Average and standard error are denoted by ‘average±standard error’. The results are based on 10 replications.

| $(m, p)$         | Algorithm [1] |
|------------------|--------------|
| (1000, 500)      | 22.3±0.1     |
| (2000, 1000)     | 40.5±0.2     |
| (5000, 1500)     | 96.5±0.3     |
| (5000, 3000)     | 99.6±0.2     |
| (10000, 3000)    | 209.1±0.4    |

D.3 Additional results for point removal experiments

Here, we conduct point removal experiments using the Gaussian synthetic datasets with $p = 30$. As Figure 6 shows, the overall tendency when $p = 30$ is similar to $p = 10$. DShapley shows a steep performance drop and other baseline methods behave as $p = 10$. In Figure 7, we conduct additional point removal experiments with the bounds in Theorem 3. Compared to DShapley, ‘Upper’ shows a slow drop but ‘Lower’ similarly behaves as DShapley, showing promising results. For instance, when $(m, p) = (2000, 30)$, Spearman’s rank correlation between ‘Lower’ and DShapley is 0.91. Lastly, we conduct additional point removal experiments with three real datasets, airfoil, boston, and diabetes. As we did in Figure 2, we first estimate covariance matrices and compute residuals to estimate DShapley. Figure 8 again shows that the steepest decrease of the relative utility for the proposed method (blue solid), compared to the other baseline methods based on Cook’s distance (green) or random deletion (magenta). Multiple real dataset analyses demonstrate the practical utility of the proposed algorithm.

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3 Compared to $D$-SHAPLEY, the proposed method is 1200 times faster when $(m, p) = (1000, 500)$. 

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20
A review of Shapley value and its uniqueness

We briefly review the Shapley axioms: symmetry, null player, and additivity. Under the axioms, we describe an equitable valuation function $\phi$. We use the same notations in Section 2.

- **Symmetry**: Let $z_i, z_j \in B$. For all $S \subseteq B \setminus \{z_i, z_j\}$, if $U(S \cup \{z_i\}) = U(S \cup \{z_j\})$, then $\phi(z_i; U, B) = \phi(z_i; U, B)$.

- **Null player**: Let $z_i \in B$. For all $S \subseteq B \setminus \{z_i, z_j\}$, if $U(S \cup \{z_i\}) = U(S)$, then $\phi(z_i; U, B) = 0$.

- **Additivity**: Let $U_1, U_2$ be two utility functions. Then for all $z \in B$ $\phi(z; U_1 + U_2, B) = \phi(z; U_1, B) + \phi(z; U_2, B)$.

Under the axioms, we provide the uniqueness theorem, quote from Osborne and Rubinstein [27, Proposition 293.1].

**Theorem 6.** Under the three Shapley axioms, the Shapley value is the unique valuation.

The original version by Shapley [31] has a slightly different conditions and we present this version, which is more reasonable to machine learning settings.
Figure 8: Relative utility (in %) as a function of the fraction of training data removed (in %) using the three real datasets, airfoil, boston, and diabetes. We remove data points from largest to lower value based on DShapley in Theorem 2.

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