RKHS-SHAP: SHAPLEY VALUES FOR KERNEL METHODS

A PREPRINT

Siu Lun Chau

Department of Statistics University of Oxford United Kingdom, OX1 3LB

Javier Gonzalez

Microsoft Research Cambridge Cambridge United Kingdom, CB1 2FB

Dino Sejdinovic

Department of Statistics University of Oxford United Kingdom, OX1 3LB

October 19, 2021

ABSTRACT

Feature attribution for kernel methods is often heuristic and not individualised for each prediction. To address this, we turn to the concept of Shapley values, a coalition game theoretical framework that has previously been applied to different machine learning model interpretation tasks, such as linear models, tree ensembles and deep networks. By analysing Shapley values from a functional perspective, we propose RKHS-SHAP, an attribution method for kernel machines that can efficiently compute both *Interventional* and *Observational Shapley values* using kernel mean embeddings of distributions. We show theoretically that our method is robust with respect to local perturbations - a key yet often overlooked desideratum for interpretability. Further, we propose *Shapley regulariser*, applicable to a general empirical risk minimisation framework, allowing learning while controlling the level of specific feature's contributions to the model. We demonstrate that the Shapley regulariser enables learning which is robust to covariate shift of a given feature and fair learning which controls the Shapley values of sensitive features.

1 Introduction

Machine learning model interpretability is critical for researchers, data scientists, and developers to explain, debug and trust their models and understand the value of their findings. A typical way to understand model performance is to attribute importance scores to each input feature [Carvalho et al.(2019)]. These scores can be computed either for an entire dataset to explain the model's overall behavior (global) or compute individually for each single prediction (local).

Understanding feature importances in reproducing kernel Hilbert space (RKHS) methods such as kernel ridge regression and support vector machines often require the study of kernel lengthscales across dimensions [Williams and Rasmussen(2006), Chapter 5]. The larger the value, the less relevant the feature is to the model. Although straight forward, this approach comes with three shortcomings: (1) It only provides global feature importances and cannot be individualised to each single prediction¹. In safety critical domain such as medicine, understanding individual prediction is arguably more important than capturing the general model performance. (2) The tuning of lengthscales often requires a user-specified grid of possible configurations and is selected using cross-validations. This pre-specification thus injects substantial amount of human bias to the explanation task. (3) Lengthscales across kernels acting on different data types, such as binary and continuous variables, are difficult to compare and interpret.

To address this problem we turn to the Shapley value (SV) [Shapley(1953)] literature, which has become central to many model explanation methods in recent years. The Shapley value was originally a concept used in game theory that involves fairly distributing credits to players working in coalition. [Štrumbelj and Kononenko(2014)] were one of the first to connect SV with machine learning explanations by casting predictions as coalition games, and features as players. Since then, a variety of SV based explanation models were proposed. For example, LINEAR-SHAP [Štrumbelj and Kononenko(2014)] for linear models, TREESHAP [Lundberg et al.(2018)] for tree ensembles and DEEPSHAP [Lundberg and Lee(2017)] for deep networks. Model agnostic methods such as DATA-SHAPLEY

¹Note that global importance does not necessarily imply local importances as discussed in [Ribeiro et al.(2016)].

[Ghorbani and Zou(2019)], SAGE [Covert et al.(2020)] and KERNELSHAP ² [Lundberg and Lee(2017)] were also proposed. However, to the best of our knowledge, an SV-based local feature attribution framework suited for kernel methods has not been proposed.

While one could still apply model-agnostic KERNELSHAP on kernel machines, we show that by representing distributions as elements in the RKHS through kernel mean embeddings [Song et al.(2013), Muandet et al.(2016)], we can compute Shapley values more efficiently by circumventing the need to sample from an estimated density. We call this approach RKHS-SHAP to distinguish it from KERNELSHAP. Through the lens of RKHS, we study Shapley values from a functional perspective and prove that our method is robust with respect to local perturbations, which is an important yet often neglected criteria for explanation models as discussed in [Hancox-Li(2020)]. In addition, a *Shapley regulariser* based on RKHS-SHAP is proposed for the empirical risk minimisation framework, allowing the modeller to control the degree of feature contribution during the learning. We also discuss its application to robust learning to covariate shift of a given feature and fair learning while controlling contributions from sensitive features. We summarise our contributions below:

- We propose RKHS-SHAP, a model specific algorithm to compute Shapley values for kernel methods.
- We prove that the corresponding Shapley values are robust to local perturbations.
- We propose a *Shapley regulariser* for the empirical risk minimisation framework, allowing the modeller to control the degree of feature contribution during the learning.

The paper is outlined as follows: In section 2 we provide an overview of Shapley values and kernel methods. In section 3 we introduce RKHS-SHAP and show robustness of the algorithm. *Shapley regulariser* is introduced in section 4. Section 5 provides extensive experiments. We conclude our work in section 6.

2 Background Materials

2.1 The Shapley Value

The Shapley value was first proposed by [Shapley(1953)] to allocate performance credit across coalition game players in the following sense: Let $\nu:\{0,1\}^d\to\mathbb{R}$ be a *coalition game* that returns a score for each coalition $S\subseteq D$, where $D=\{1,...,d\}$ represents a set of players. Assuming the grand coalition D is participating and one wished to provide the i^{th} player with a fair allocation of the total profit $\nu(D)$, how should one do it? Surely this is related to each player's marginal contribution to the profit with respect to a coalition S, i.e. $\nu(S\cup i)-\nu(S)$. [Shapley(1953)] proved that there exists a unique combination of marginal contributions that satisfies a set of favorable and fair game theoretical axioms, commonly known as efficiency, null player, symmetry and additivity. This unique combination of contributions is later denoted as the Shapley value. Formally, given a coalition game ν , the Shapley value for player i is computed as the following,

$$\phi_i(v) = \frac{1}{d} \sum_{S \subseteq D \setminus \{i\}} {d-1 \choose |S|}^{-1} \Big(\nu(S \cup i) - \nu(S) \Big). \tag{1}$$

Choosing ν for ML explanation In recent years, the Shapley value concept has become popular for feature attribution in machine learning. SHAP [Lundberg and Lee(2017)], SHAPLEY EFFECT [Song et al.(2016)], DATA-SHAPLEY [Ghorbani and Zou(2019)] and SAGE [Covert et al.(2020)] are all examples that cast model explanations as coalition games by choosing problem specific value functions ν . Denote f as the machine learning model mapping from an instance space $\mathcal X$ to a label space $\mathcal Y$. Value functions for local attribution on observation x often take the form of the expectation of f with respect to reference distribution $r(X_{S^c}|x_S)$, where S is some selected set of features, such that:

$$\nu_{x,S}(f) = \mathbb{E}_{r(X_{S^c}|x_S)}[f(\{x_S, X_{S^c}\})]$$
 (2)

 $\{x_S, X_{S^c}\}$ denotes the concatenation of the arguments. We have written f as the main argument of ν to highlight its interpretation as a functional indexed by local observation x and coalition S. When r is set to be marginal distribution, i.e $r(X_{S^c}|x_S) = p(X_{S^c})$, the value function is denoted as the *Interventional value function* by [Janzing et al.(2020)]. Observational value function [Frye et al.(2020)], on the other hand, set the reference distribution to be conditional distribution $p(X_{S^c}|X_S=x_S)$. In fact, these methods can be seen as examples of removal-based explanations [Covert et al.(2020)] since certain features are removed via integration to understand their impact on the model. See Figure 1 for an illustration of how Shapley values are adapted to model interpretation tasks.

²The kernel in KERNELSHAP refers to the estimation procedure is not related to RKHS kernel methods.

$\phi_{x,i}(f) = \frac{1}{d} \sum_{S \subseteq D \setminus \{i\}} \binom{d-1}{|S|}^{-1} \left(\nu_{x,S \cup i}(f) - \nu_{x,S}(f)\right) \\ \frac{x}{i} \qquad \begin{array}{c|c} \text{local observation} \\ \hline i & \text{feature to attribute} \\ \hline f & \text{machine learning model} \\ \hline D & \text{feature set } \{1, \dots, d\} \\ \hline \nu_{x,S} & \text{value functional} \\ \hline \phi_{x,i} & \text{Shapley functional (See Prop. 5)} \\ \end{array}$

Figure 1: The Shapley value formulation for machine learning model interpretation

Definition 1. Given model f, local observation x and a coalition set $S \subseteq D$, the Interventional and Observational value functions are denoted by $\nu_{x,S}^{(I)}(f) := \mathbb{E}[f(\{x_S, X_{S^c}\})]$ and $\nu_{x,S}^{(O)}(f) := \mathbb{E}[f(\{x_S, X_{S^c}\})|X_S = x_S]$.

The right choice of ν has been a long-standing debate in the community. While [Janzing et al.(2020)] argued from a causal perspective that $\nu_{x,f}^{(I)}$ is the correct notion to represent missingness of features in an explanation task, [Frye et al.(2020)] argued that computing marginal expectation ignores feature correlation and leads to unrealistic results since one would be evaluating the value function outside the data-manifold. This controversy was further investigated by [Chen et al.(2020)], where they argued that the choice of ν is application dependent and the two approaches each lead to an explanation that is either true to the model (marginal expectation) or true to the data (conditional expectation). [Chen et al.(2020)] called the former as Interventional Shapley value and the latter as Observational Shapley value. When the context is clear, we denote the Shapley value of the i^{th} feature of data x at f as $\phi_{x,i}(f)$ and use a superscript to indicate whether it is Interventional, $\phi_{x,i}^{(I)}(f)$ or Observational $\phi_{x,i}^{(O)}(f)$.

2.1.1 Computing Shapley values

While Shapley values can be estimated directly from Eq. (1) using a sampling approach [Štrumbelj and Kononenko(2014)], [Lundberg and Lee(2017)] proposed KERNELSHAP, a more efficient algorithm for estimating Shapley values in high dimensional feature spaces by casting Eq. (1) as a weighted least square problem. Similar to LIME [Ribeiro et al.(2016)], for each data x, KERNELSHAP places a linear model $u_x(S) = \beta_{x,0} + \sum_{i \in S} \beta_{x,i}$ to explain $\nu_x(S)$ and solves the following regression problem:

$$\min_{\beta_{x,0},\dots,\beta_{x,d}} \sum_{S \subseteq D} w(S) \left(u_x(S) - \nu_x(S) \right)^2 \tag{3}$$

where $w(S) = \frac{d-1}{\binom{d}{|S|}|S|(d-|S|)}$ is a carefully chosen weighting such that the recovered regression coefficients equate Shapley values. In particular, one set $w(\varnothing) = w(D) = \infty$ to effectively enforce constraints $\beta_{x,0} = \nu_x(\varnothing)$ and $\sum_{i \in D} \beta_{x,i} = \nu_x(D) - \nu_x(\varnothing)$.

Denoting each subset $S \subseteq D$ using the corresponding binary vector $\mathbf{z} \in \{0,1\}^d$, and with an abuse of notation by setting $\nu(\mathbf{z}) := \nu(S)$ and $w(\mathbf{z}) := w(S)$ for $S = \{j : \mathbf{z}[j] = 1\}$, we can express the Shapley values $\boldsymbol{\beta}_x := [\beta_{x,0},...,\beta_{x,d}]$ as $\boldsymbol{\beta}_x = (Z^\top W Z)^{-1} Z^\top W \mathbf{v}_x$ where $Z \in \mathbb{R}^{2^d \times d}$ is the binary matrices with columns $\{\mathbf{z}_i\}_{i=1}^{2^d}$, W is the diagonal matrix with entries $w_{ii} = w(\mathbf{z}_i)$ and $\mathbf{v}_x := \{\nu_x(\mathbf{z}_i)\}_{i=1}^{2^d} \in \mathbb{R}^{2^d \times 1}$ the vector of evaluated value functions, which is often estimated using sampling and data imputations. We explain this in detail later in Section 3. In practice, instead of evaluating at all 2^d combinations, one would subsample the coalitions $z \sim w(z)$ for computational efficiency.

2.1.2 Model specific Shapley methods

KERNELSHAP provides efficient model-agnostic estimations of Shapley values. However, by leveraging additional structural knowledge about specific models, one could further improve computational performance. This leads to a variety of model-specific approximations. For example, LINEARSHAP [Štrumbelj and Kononenko(2014)] explain linear models using model coefficients directly. TREESHAP [Lundberg et al.(2018)] provides an exponential reduction in complexity compared to KERNELSHAP by exploiting the tree structure. DEEPSHAP [Lundberg and Lee(2017)], on the other hand, combines DEEPLIFT [Shrikumar et al.(2017)] with Shapley values and uses the compositional nature of deep networks to improve efficiencies. However, to the best of our knowledge, a kernel method specific Shapley value approximation has not been studied. Later in Section 3, we will show that kernel methods speeds up KERNELSHAP by estimating value functions analytically, thus circumventing the need for sampling and data imputations from an estimated density.

Related work on kernel-based Shapley methods The closest work to ours is from [Da Veiga(2021)], where the author proposed using kernel-based distributional metric such as *Maximum Mean Discrepancy* as the coalition game to compute the Shapley effect [Song et al.(2016)]. The main difference between our work and theirs is that they focused on *global* sensitivity analysis while ours is on crediting *local* feature importance. This leads to different choices of value functions and estimation approaches thus leading to completely different algorithms.

2.2 Kernel Methods

Kernel methods are one of the pillars of machine learning, as they provide flexible yet principled ways to model complex functional relationships and come with well-established statistical properties and theoretical guarantees.

Empirical Risk Minimisation Let $\mathcal{X} \subseteq \mathbb{R}^d$ be an instance space, \mathcal{Y} a label space, and p(x,y) a probability density on $\mathcal{X} \times \mathcal{Y}$. Recall in the supervised learning framework, we are learning a function $f: \mathcal{X} \to \mathcal{Y}$ from a hypothesis space \mathcal{H} , such that given training set $(\mathbf{x}, \mathbf{y}) = \{(x_i, y_i)\}_{i=1}^n$ sampled identically and independently from p, the following empirical risk is minimised:

$$f^* = \arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(y_i, f(x_i)) + \lambda_f \Omega(f)$$
(4)

where $\ell: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ is the loss function, $\Omega: \mathcal{H} \to \mathbb{R}$ a regularisation function and λ_f a scalar controlling the level of regularisation. Denote $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ a positive definite kernel with feature map ψ_x for input $x \in \mathcal{X}$ and \mathcal{H}_k the corresponding RKHS. If we pick \mathcal{H}_k as our hypothesis space, then the *Representer theorem* [Steinwart and Christmann(2008)] tells us that the optimal solution takes the form of $f^* = \sum_{i=1}^n \alpha_i k(\cdot, x_i) = \Psi_{\mathbf{x}} \alpha$, where $\Psi_{\mathbf{x}} = [\psi_{x_1} \dots \psi_{x_n}]$ is the feature matrix defined by stacking feature maps along columns. If ℓ is the squared loss then the above optimisation is known as kernel ridge regression and α can be recovered in closed form $\alpha = (\mathbf{K}_{\mathbf{x}\mathbf{x}} + \lambda_f I)^{-1}\mathbf{y}$, where $\mathbf{K}_{\mathbf{x}\mathbf{x}} = \Psi_{\mathbf{x}}^{\top}\Psi_{\mathbf{x}}$ is the kernel matrix. If ℓ is the logistic loss, then the problem is known as kernel logistic regression, and α can be obtained using gradient descent.

2.2.1 Kernel embedding of distributions

An essential component for RKHS-SHAP is the embedding of both marginal and conditional distribution of features into the RKHS, thus allowing one to estimate the value function analytically.

Kernel mean embeddings (KME) of distributions provide a powerful framework for presenting and manipulating probability distributions [Song et al.(2013), Muandet et al.(2016)]. Formally, the kernel mean embedding (KME) of a marginal distribution P_X is defined as $\mu_X := \mathbb{E}_X[\psi_X] = \int_{\mathcal{X}} \psi_x dP_X(x)$ and the empirical estimate can be obtained as $\hat{\mu} := \frac{1}{n} \sum_{i=1}^n \psi_{x_i}$. Furthermore, given another kernel $g: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ with the corresponding feature map ψ_Y of RKHS \mathcal{H}_g , the conditional mean embedding (CME) of the conditional distribution $P_{Y|X=x}$ is defined as $\mu_{Y|X=x} := \mathbb{E}[\psi_Y|X=x] = \int_{\mathcal{Y}} \psi_y dP_{Y|X=x}(y)$.

In fact, [Song et al.(2013)] showed that we could associate a conditional mean operator (CMO) $C_{Y|X}:\mathcal{H}_k\to\mathcal{H}_g$ such that $\mu_{Y|X=x}=C_{Y|X}\psi_x$. The CMO can be written in terms of covariance operators: $C_{Y|X}=C_{YX}C_{XX}^{-1}$ where $C_{YX}:=\mathbb{E}_{Y,X}[\psi_Y\otimes\psi_X]$ and $C_{XX}:=\mathbb{E}_X[\psi_X\otimes\psi_X]$. As a result, the finite sample estimator of $C_{Y|X}$ can be written as:

$$\hat{C}_{Y|X} = \frac{1}{n} \Psi_{\mathbf{y}} \Psi_{\mathbf{x}}^{\top} \left(\frac{1}{n} \Psi_{\mathbf{x}} \Psi_{\mathbf{x}}^{\top} + \eta I \right)^{-1}$$
(5)

$$= \Psi_{\mathbf{y}} (\mathbf{K}_{\mathbf{x}\mathbf{x}} + n\eta I)^{-1} \Psi_{\mathbf{x}}^{\top}$$
 (6)

where $\Psi_{\mathbf{y}} := [\psi_{y_1}...\psi_{y_n}]$ and $\Psi_{\mathbf{x}} := [\psi_{x_1}...\psi_{x_n}]$ are feature matrices and $\eta > 0$ is the regularisation parameter ensuring the operators are globally defined.

In fact, when using finite-dimensional feature maps, such as in the case with running Random Fourier Features [Rahimi et al.(2007)] and Nyström methods [Yang et al.(2012)] for scalability, one could choose to evaluate the empirical CMO using Eq(5), which reduces the computational complexity from $\mathcal{O}(n^3)$ to $\mathcal{O}(b^3) + \mathcal{O}(b^2n)$ where b is the dimension of the feature map and often can be chosen much smaller than n [Li et al.(2019a)].

3 RKHS-SHAP

While KERNELSHAP is model agnostic, by restricting our attention to the class of kernel methods, faster Shapley value estimation can be derived. In the following, we will lay out the disadvantage of existing sampling and data imputation

approach and show that by estimating the value functionals as elements in the RKHS, we can circumvent the need for sampling – thus improving the computational efficiency in the estimation.

Estimating value functions by sampling [Chen et al.(2020)] defined *Interventional Shapley values* (ISVs) and *Observational Shapley values* (OSVs) as Shapley values obtained with respect to the following functionals,

$$\nu_{x,S}^{(I)}(f) = \mathbb{E}[f(\{x_S, X_{S^c}\})] \tag{7}$$

$$\nu_{x,S}^{(O)}(f) = \mathbb{E}[f(\{x_S, X_{S^c}\}) | X_S = x_S]$$
(8)

Estimating $\nu_{x,S}^{(O)}(f)$ is typically much harder than $\nu_{x,S}^{(I)}(f)$ as it requires integration with respect to the unknown conditional density $p(X_{S^c}|X_S)$. Therefore, estimating OSVs often boils down to a two-stage approach: (1) Conditional density estimation and (2) Monte Carlo averaging over imputed data. [Aas et al.(2019)Aas, Jullum, and Løland] considered using multivariate Gaussian and Gaussian Copula for density estimation while [Frye et al.(2020)] used a deep unsupervised network. While deep networks do not pose any parametric assumptions on the density, it is known that deep density estimation requires large amounts of training data and is often prone to overfitting [Schuster et al.(2020)].

Once the conditional density $p(X_{S^c}|X_S)$ for each $S\subseteq D$ is estimated, the observational value function at the i^{th} observation x_i can then be computed by taking averages of m Monte Carlo samples from the estimated conditional density, i.e. $\frac{1}{m}\sum_{j=1}^m f(\{x_{iS},x_{jS^c}\})$ where $\{x_{iS},x_{jS^c}\}$ is the concatenation of x_{iS} with the j^{th} sample x_{jS^c} from $p(X_{S^c}|X_S=x_{iS})$. Note further that the Monte Carlo samples cannot be reused for another observation x_k as their conditional densities are different. In other words, $n\times m$ Monte Carlo samples are required for each coalition S if one wishes to compute Shapley values for all n observations. This is clearly not desirable. In the spirit of Vapnik's principle³, as our goal is to estimate conditional expectations that lead to Shapley values, we are not going to solve a harder and more general problem of conditional density estimation as an intermediate step, but instead utilise the arsenal of kernel methods to estimate the conditional expectations directly.

Estimating value functions using mean embeddings If our model f lives in \mathcal{H}_k , both the marginal and conditional expectation can be estimated analytically without any sampling or density estimation. We first show that the Riesz representations [Paulsen and Raghupathi(2016)] of both *Interventional* and *Observational value functionals* exist and are well-defined in \mathcal{H}_k . In the following, for simplicity, we will denote the functional and its corresponding Riesz representer using the same notation. For example, we will write $\nu_{x,S}(f) = \langle f, \nu_{x,S} \rangle_{\mathcal{H}_k}$ when the context is clear. All proofs of this paper can be found in the supplementary material.

Proposition 2 (Riesz representations of value functionals). Denote k as the product kernel of D bounded kernels $k_d: \mathcal{X}^{(d)} \times \mathcal{X}^{(d)} \to \mathbb{R}$, where $\mathcal{X}^{(d)}$ is the domain of the d^{th} feature. Riesz representations of the Interventional and Observational value functionals exists and can be written as $\nu_{x,S}^{(I)} = \psi_{x_S} \otimes \mu_{X_{S^c}}$ and $\nu_{x,S}^{(O)} = \psi_{x_S} \otimes \mu_{X_{S^c}|X_S=x_S}$, where $\psi_{x_S} := \bigotimes_{i \in S} \psi_{x^{(i)}}$, $\mu_{X_{S^c}} := \mathbb{E}[\bigotimes_{i \in S^c} \psi_{x^{(i)}}]$ and $\mu_{X_{S^c}|X_S=x_S} := \mathbb{E}[\bigotimes_{i \in S^c} \psi_{x^{(i)}}|X_S=x_S]$.

The corresponding finite sample estimators $\hat{\nu}_{x,S}^{(I)}$ and $\hat{\nu}_{x,S}^{(O)}$ are then obtained by replacing the corresponding KME and CME components with their empirical estimators. As a result, given $f^* = \Psi_{\mathbf{x}} \alpha$ trained on dataset (\mathbf{x}, \mathbf{y}) , Eq(7) and Eq(8) can now be estimated analytically since $\hat{\nu}_{x,S}^{(I)}(f^*) = \langle f^*, \psi_{x_S} \otimes \hat{\mu}_{X_{S^c}} \rangle$ and $\hat{\nu}_{x,S}^{(O)}(f^*) = \langle f^*, \psi_{x_S} \otimes \hat{\mu}_{X^{S^c}|X_S=x_S} \rangle$. This corresponds to the direct non-parametric estimators of value functions given in the following Proposition, which circumvent the need for sampling or density estimation.

Proposition 3. Given $\mathbf{x}' \in \mathbb{R}^{n'}$ a vector of instances and $f = \Psi_{\mathbf{x}} \alpha$, the empirical estimates of $\nu_{\mathbf{x}',S}^{(I)}(f)$ and $\nu_{\mathbf{x}',S}^{(O)}(f)$ can be computed as,

$$\hat{\nu}_{\mathbf{x}',S}^{(I)}(f) = \boldsymbol{\alpha}^{\top} \mathcal{K}_{\mathbf{x}',S}^{(I)} \qquad \hat{\nu}_{\mathbf{x}',S}^{(O)}(f) = \boldsymbol{\alpha}^{\top} \mathcal{K}_{\mathbf{x}',S}^{(O)}$$

$$(9)$$

where $\mathcal{K}_{\mathbf{x}',S}^{(I)} = \mathbf{K}_{\mathbf{x}_S \mathbf{x}_S'} \odot \frac{1}{n} \operatorname{diag}(\mathbf{K}_{\mathbf{x}_{S^c} \mathbf{x}_{S^c}}^{\top} \mathbf{1_n}) \mathbf{1_n} \mathbf{1_n}^{\top}$ and $\mathcal{K}_{\mathbf{x}',S}^{(O)} = \mathbf{K}_{\mathbf{x}_S \mathbf{x}_S'} \odot \Xi_S \mathbf{K}_{\mathbf{x}_S \mathbf{x}_S'}$, $\mathbf{1_n}$ is the all-one vector with length n, \odot the Hadamard product and $\Xi_S = \mathbf{K}_{\mathbf{x}_{S^c} \mathbf{x}_{S^c}} (\mathbf{K}_{\mathbf{x}_S \mathbf{x}_S} + n\eta I)^{-1}$.

Finally, to obtain the Shapley values with these value functions, we deploy the same least square approach as KER-NELSHAP.

Proposition 4 (RKHS-SHAP). Given $f \in \mathcal{H}_k$ and a value functional ν , Shapley values $\mathbf{B} \in \mathbb{R}^{d \times n}$ for all d features and all n input \mathbf{x} can be computed as $\mathbf{B} = (Z^\top W Z)^{-1} Z^\top W \hat{\mathbf{V}}$ where $\hat{\mathbf{V}}_{i,:} = \langle f, \hat{\nu}_{\mathbf{x}, S_i} \rangle$.

³When solving a given problem, try to avoid solving a more general problem as an intermediate step. [Vapnik(1995), Section 1.9]

3.1 Robustness of RKHS-SHAP

Robustness of interpretability methods is important from both epistemic and ethical perspective as discussed in [Hancox-Li(2020)]. On the other hand, [Alvarez-Melis and Jaakkola(2018)] showed empirically that Shapley methods when used with complex non-linear black-box models such as neural networks, yield explanations that vary considerably for some neighboring inputs, even if the deep network gives similar predictions at those neighborhood. In light of this, we analyse the Shapley values obtained from our proposed RKHS-SHAP and show that they are robust. To illustrate this, we first formally define the *Shapley functional*,

Proposition 5 (Shapley functional). Given a value functional ν indexed by input x and coalition S, the Shapley functional $\phi_{x,i}: \mathcal{H}_k \to \mathbb{R}$ such that $\phi_{x,i}(f)$ is the i^{th} Shapley values of input x on model f, has the following Reisz representation in the RKHS: $\phi_{x,i} = \frac{1}{d} \sum_{S \subseteq D \setminus \{i\}} {d-1 \choose |S|}^{-1} (\nu_{x,S \cup i} - \nu_{x,S})$

Analogously, we denote $\phi_{x,i}^{(I)}$ and $\phi_{x,i}^{(O)}$ as the *Interventional Shapley functional* (ISF) and *Observational Shapley functional* respectively (OSF).

Note that the functional depends only on data and the RKHS chosen, and not on the specific function f that it will be applied to. Using the functional formalism, we now show that given $f \in \mathcal{H}_k$, when $||x - x'||^2 \le \delta$ for $\delta > 0$, the difference in Shapley values at x and x' will be arbitrarily small for all features i.e. $|\phi_{x,i}(f) - \phi_{x',i}(f)|$ is small $\forall i \in D$. This corresponds to the following,

$$|\phi_{x,i}(f) - \phi_{x',i}(f)|^2 = |\langle f, \phi_{x,i} - \phi_{x',i} \rangle|^2$$
(10)

$$\leq ||f|||_{\mathcal{H}_{\nu}}^{2} ||\phi_{x,i} - \phi_{x',i}||_{\mathcal{H}_{\nu}}^{2} \tag{11}$$

where we use Cauchy-Schwarz for the last line. Therefore, for a given f with fix RKHS norm, the key to show robustness lies into bounding the Shapley functionals as follows:

Theorem 6 (Bounding Shapley functionals). Let k be a product kernel with d bounded kernels $|k^{(i)}(x,x)| \leq M$ for all $i \in D$. Denote $||.||_{op}$ the operator norm, $M_{\mu} := \sup_{S \subseteq D} M^{|S|}, M_C := \sup_{S \subseteq D} ||C_{X_{S^c}|X_S}||_{op}^2$ and $L_{\delta} = \sup_{S \subseteq D} ||\psi_{x_S} - \psi_{x_S'}||_{\mathcal{H}_k}^2$. Let $\delta > 0$, assume $|x^{(i)} - x^{(i)'}|^2 \leq \delta$ for all features $i \in D$, then differences of the Interventional and Observational Shapley functionals for feature i at observation x, x' can be bounded as $||\phi_{x,i}^{(I)} - \phi_{x',i}^{(I)}||_{\mathcal{H}_k}^2 \leq 2M_{\mu}L_{\delta}$ and $||\phi_{x,i}^{(O)} - \phi_{x',i}^{(O)}||_{\mathcal{H}_k}^2 \leq 4M_CM_{\mu}L_{\delta}$. If k is the RBF kernel with lengthscale l, then

$$||\phi_{x,i}^{(I)} - \phi_{x',i}^{(I)}||_{\mathcal{H}_k}^2 \le 4\left(1 - \exp\left(\frac{-d\delta}{2l^2}\right)\right)$$
(12)

$$||\phi_{x,i}^{(O)} - \phi_{x',i}^{(O)}||_{\mathcal{H}_k}^2 \le 8M_C \left(1 - \exp\left(\frac{-d\delta}{2l^2}\right)\right)$$
(13)

Therefore, as long as $||f||_{\mathcal{H}_k}$ is small, RKHS-SHAP will return robust Shapley values with respect to small perturbations. Recall Shapley functionals do not depend on f and can be estimated separately purely based on data. In the next section we will see that the functional itself can be used to aid in learning of f and allow enforcing particular additional structural constraints on f via an additional regularisation term.

4 Shapley regularisation

Regularisation is popular in machine learning because it allows inductive bias to be injected to learn functions with specific properties. For example, classical L_1 and L_2 regularisers are used to control the sparsity and smoothness of model parameters. Manifold regularisation [Belkin et al.(2006)Belkin, Niyogi, and Sindhwani], on the other hand, exploits the geometry of the distribution of unlabelled data to improve learning in a semi-supervised setting, whereas [Pérez-Suay et al.(2017)] and [Li et al.(2019b)] adopted a kernel dependence regulariser to learn functions for fair regression and fair dimensionality reduction. In the following, we propose a new *Shapley regulariser* based on the Shapley functionals, which allows learning while controlling the level of specific feature's contributions to the model.

Formulation Let A be a specific feature whose contribution we wish to regularise, f the function we wish to learn, and $\phi_{x_i,A}(f)$ the Shapley value of A at a given observation x_i . Our goal is to penalise the mean squared magnitude of $\{\phi_{x_i,A}(f)\}_{i=1}^n$ in the ERM framework, which corresponds to,

$$\min_{f \in \mathcal{H}_k} \sum_{i=1}^n \ell(y_i, f(x_i)) + \lambda_f ||f||_{\mathcal{H}_k}^2 + \frac{\lambda_S}{n} \sum_{i=1}^n |\phi_{x_i, A}(f)|^2$$

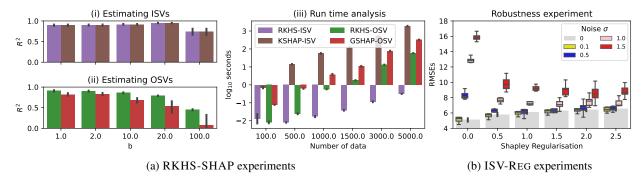


Figure 2: (a) RKHS-SHAP: Estimation of Shapley values using data from the Banana distribution. Run time analysis is also reported. (b) ISV-REG: RMSEs of f_{reg} on noisy test data at different noise level σ' . All scores are averaged over 10 runs and 1 sd is reported.

where ℓ is some loss function and λ_f and λ_S control the level of regularisation. If we replace the population Shapley functional with the finite sample estimate, and utilise the Representer theorem, we can rewrite the optimisation in terms of α .

Proposition 7. The above optimisation can be rewritten as,

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^n} \sum_{i=1}^n \ell(y_i, \mathbf{K}_{x_i \mathbf{x}} \boldsymbol{\alpha}) + \lambda_f \boldsymbol{\alpha}^\top \mathbf{K}_{\mathbf{x} \mathbf{x}} \boldsymbol{\alpha} + \frac{\lambda_S}{n} \boldsymbol{\alpha}^\top \Gamma_A \Gamma_A^\top \boldsymbol{\alpha}$$

To regularise the Interventional SVs (ISV-REG) of A, we set $\Gamma_A = \frac{1}{J} \sum_{j=1}^J \mathcal{K}_{\mathbf{x},S_j \cup A}^{(I)} - \mathcal{K}_{\mathbf{x},S_j}^{(I)}$ where S_j 's are coalitions sampled from $p_{SV}(S) = \frac{1}{d} {d-1 \choose |S|}^{-1}$. For regularising Observational SVs (OSV-REG), we set $\Gamma_A = \frac{1}{J} \sum_{j=1}^J \mathcal{K}_{\mathbf{x},S_j \cup A}^{(O)} - \mathcal{K}_{\mathbf{x},S_j}^{(O)}$.

In particular, closed form optimal dual weights $\alpha = \left(\mathbf{K}_{\mathbf{x}\mathbf{x}}^2 + \lambda_f \mathbf{K}_{\mathbf{x}\mathbf{x}} + \frac{\lambda_S}{n} \Gamma_A \Gamma_A^{\mathsf{T}}\right)^{-1} \mathbf{K}_{\mathbf{x}\mathbf{x}} \mathbf{y}$ can be recovered when ℓ is the squared loss.

Choice of regularisation Similar to the feature attribution problem, *the choice of regularising against ISVs or OSVs is application dependent* and boils down to whether one wants to take the correlation of A with other features into account or not.

ISV-REG ISV-REG can be used to protect the model when covariate shift of variable A is expected to happen at test time and one wishes to downscale A's contribution during training instead of completely removing this (potentially useful) feature. Such situation may arise if, e.g., a different measurement equipment or process is used for collecting observations of A during test time. ISV is well suited for this problem as dependencies across features will be broken by the covariate shift at test time.

OSV-REG On the other hand, OSV-REG can find its application in fair learning – learning a function that is fair with respect to some sensitive feature A. There exist a variety of fairness notions one could consider, such as, e.g. Statistical Parity, Equality of Opportunity and Equalised Odds [Corbett-Davies and Goel(2018)]. In particular, we consider the fairness notion recently explored in the literature [Jain et al.(2020), Mase et al.(2021)] that uses Shapley values, which are becoming a bridge between Explainable AI and fairness, given that they can detect biased explanations from biased models. In particular, [Jain et al.(2020)] illustrated that if a model is fair against a sensitive feature A, A should have neither a positive or negative contribution towards the prediction. This corresponds to A having SVs with negligible magnitudes. As contributions of A might enter the model via correlated features, it is important to take feature correlations into account while regularising. Hence, it is natural to deploy OSV-REG for fair learning.

5 Experiments

We investigate the properties of RKHS-SHAP and Shapley regularisers on four synthetic experiments. In the first two experiments, we evaluate RKHS-SHAP methods against benchmarks on estimating Interventional and Observational SVs on a Banana-shaped distribution with nonlinear dependencies [Sejdinovic et al.(2014)]. The setup allows us to

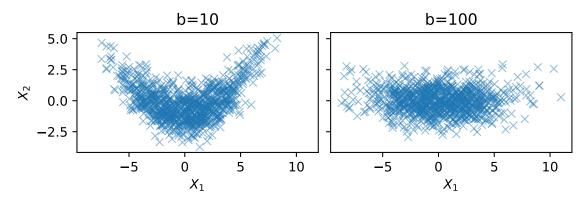


Figure 3: Illustration of $\mathcal{B}(b^{-1}, 10)$ at b = 10 and 100

obtain closed-form expressions for the ground truth ISVs and OSVs, yet the conditional distributions among features are challenging to estimate using any standard parameteric density estimation methods. We also present a run time analysis to demonstrate empirically that mean embedding based approaches are significantly more efficient than sampling based approaches. Finally, the last two experiments are applications of Shapley regularisers in robust modelling to covariate shifts and fair learning with respect to sensitive feature.

In the following, we denote RKHS-OSV and RKHS-ISV as the OSV and ISV obtained from RKHS-SHAP. As benchmark, we implement the model agnostic sampling-based algorithm KERNELSHAP from the Python package **shap**⁴. We denote the ISV obtained from KERNELSHAP as KSHAP-ISV. As **shap** does not offer model-agnostic OSV algorithm, we implement the approach from [Aas et al.(2019)Aas, Jullum, and Løland] (described in Section 3), where OSVs are estimated using Monte Carlo samples from fitted multivariate Gaussians. We denote this approach as GSHAP-OSV. We fit a kernel ridge regression on each of our experiments. Lengthscales of the kernel are selected using median heuristic [Flaxman et al.(2016)] and regularisation parameters are selected using cross-validation. Further implementation details and real world data illustrations are included in the supplementary material. All code and implementations are made publicly available ⁵.

5.1 RKHS-SHAP experiments

Experiment 1: Estimating Shapley values from Banana data We consider the following 2d-Banana distribution $\mathcal{B}(b^{-1},v)$ from [Sejdinovic et al.(2014)]: Sample $Z \sim N(0,\operatorname{diag}(v,1))$ and transform the data by setting $X_1 = Z_1$ and $X_2 = b^{-1}(Z_1^2 - v) + Z_2$. Regression labels are obtained from $f_{\text{truth}}(X) = b^{-1}(X_1^2 - v) + X_2$. This formulation allows us to compute the true ISVs and OSVs in closed forms, i.e $\phi_{X,1}^{(I)}(f_{\text{truth}}) = b^{-1}(X_1^2 - v)$, $\phi_{X,2}^{(I)}(f_{\text{truth}}) = X_2$, $\phi_{X,1}^{(O)}(f_{\text{truth}}) = \frac{1}{2}(3b^{-1}(X_1^2 - v) - X_2)$ and $\phi_{X,2}^{(O)}(f_{\text{truth}}) = \frac{1}{2}(3X_2 - b^{-1}(X_1^2 - v))$. In the following we will simulate 1000 data points from $\mathcal{B}(b^{-1},10)$ with $b \in [1,10,20,50,100]$, where smaller values of b correspond to more nonlinearly elongated distributions. See Figure 3 for visualisation of the effect of b on X. We choose R^2 as our metric since the true Shapley values for each experiment are scaled according to b.

Figure 2a(i) and 2a(ii) demonstrate R^2 scores of estimated ISVs and OSVs in contrast with groundtruths SVs across different configurations. We see that RKHS-ISV and KSHAP-ISV give exactly the same R^2 scores across configurations. This is not surprising as the two methods are mathematically equivalent. While in KSHAP-ISV one averages over evaluated $\{f(x_j')\}$ with x_j' being the imputed data, RKHS-ISV aggregated feature maps of the imputed data first before evaluating at f, i.e $\sum_{j=1} f(x_j') = \langle f, \sum_{j=1} \phi(x_j') \rangle_{\mathcal{H}_k} = \langle f, \hat{\mu}_X \rangle_{\mathcal{H}_k}$. However, it is this subtle difference in the order of operations contribute to a significant computational speed difference as we later show in Experiment 2. In the case of estimating OSVs, we see RKHS-OSV is consistently better than GSHAP-OSV at all configurations. This highlights the merit of RKHS-OSV as no density estimation is needed, thus avoiding any potential misspecification which happens in GSHAP-OSV.

Experiment 2: Run time analysis In this experiment we sample n data points from $\mathcal{B}(1,10)$ where $n \in [100, 500, 1000, 1500, 3000, 5000]$ and record the \log_{10} seconds required to complete each algorithm. In practice, as the software documentation of **shap** suggests, one is encouraged to subsample their data before passing to the

⁴https://github.com/slundberg/shap

⁵https://anonymous.4open.science/r/RKHS-SHAP/

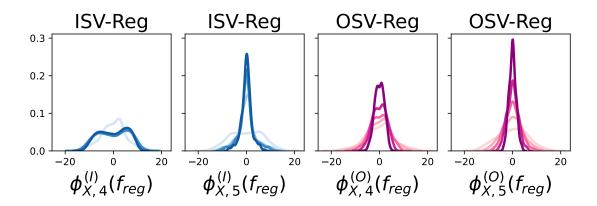


Figure 4: OSV-REG experiment: Distributions of ISVs and OSVs of sensitive feature X_5 and correlated feature X_4 obtained from ISV-REG and OSV-REG at different regularisation parameters. Colour intensity represents the strength of regularisation.

KERNELSHAP algorithm as the background sampling distribution to avoid slow run time. As this approach speeds up computation at the expense of estimation accuracy since less data is used, for fair comparison with our RKHS-SHAP method which utilises all data, we pass the whole training set to the KERNELSHAP algorithm. Figure 2a(iii) illustrates the run time across methods. We note that the difference in runtime between the two sampling based methods KSHAP-ISV and GSHAP-OSV can be attributed to a different software implementation, but we observe that they are both significantly slower than RKHS-ISV and RKHS-OSV. RKHS-OSV is slower than RKHS-ISV as it involves matrix inversion when computing the empirical CME. In practice, one can trivially subsample data for RKHS-SHAP to achieve further speedups like in the **shap** package, but one can also deploy a range of kernel approximation techniques as discussed in Section 2.2.1.

5.2 Shapley regularisation experiments

For the last two experiments we will simulate 1000 samples from $X \sim N(0, \Sigma)$ with $\operatorname{diag}(\Sigma) = \mathbf{1_5}$ and $\Sigma_{4,5} = \Sigma_{5,4} = 0.9$, 0 otherwise, therefore feature X_4 and X_5 will be highly correlated. We set our regression labels as $f_{\text{true}}(x) = x^{\top}\beta$ with $\beta = [1, 2, 3, 4, 15]$, enforcing X_5 to be the most influential feature. We use 70% of our data for training and 30% for testing.

Experiment 3: Protection against covariate shift using ISV-REG For this experiment, we inject extra mean zero Gaussian noise to the most influential feature X_5 in the testing set, i.e $X_5' = X_5 + \sigma' N(0,1)$ for $\sigma' \in [0,0.1,0.5,1,1.5]$. We assume that there is an expectation for covariate shift in X_5 to occur at test time, due to e.g. a change in measurement precision – hence, we train our model f_{reg} using ISV-REG at different regularisation level λ_s for $\lambda_s \in [0,0.5,1,1.5,2,2.5]$. We then compare RMSEs when no covariate shift is present ($\sigma' = 0$) against RMSEs at different noise levels. The results are shown in Figure 2b. We see that when no regularisation is applied, RMSEs increase rapidly as σ' increases, indicating our standard unprotected kernel ridge regressor is sensitive to noises from X_5' . As Shapley regularisation parameter increases, the RMSE of the noiseless case gradually increases too, but RMSEs of the noisy data are much closer to the noiseless case, exhibiting robustness to the covariate shift.

Experiment 4: Fair learning with OSV-REG At last, we demonstrate the use of Shapley regulariser to enable fair learning. In this context, as we will see OSV-REG is the appropriate regulariser. Consider X_5 as some sensitive feature which we would like to minimise its contribution during the learning of f. Recall X_4 is highly correlated to X_5 so it contains sensitive information from X_5 as well. Figure 4 demonstrates how distributions of ISVs and OSVs of X_4 and X_5 changes as λ_s increases. As regularisation increases, the SVs of X_5 becomes more centered at 0, indicating lesser contribution to the model f_{reg} . Similar behavior can be seen from the distribution of $\phi_{X,4}^{(O)}(f_{\text{reg}})$ but not from $\phi_{X,4}^{(I)}$. This illustrates how ISV-REG will propagate unfairness through correlated feature X_4 while OSV-REG can take them into account by minimising the contribution of sensitive information during learning.

6 Conclusion and future directions

Explainable AI is an important field allowing humans to better understand and interpret black box machine learning models and Shapley values are one of key tools of explainable AI. In this work, we proposed a more accurate and more efficient algorithm to compute Shapley values for kernel methods, termed RKHS-SHAP. We proved that the corresponding local attributions are robust to local perturbations. Furthermore, we proposed the Shapley regulariser which allows learning while controlling specific feature contribution to the model. We suggested two applications of this regulariser and concluded our work with extensive experiments demonstrating different aspects of our contributions.

While our methods currently only are applicable to functions arising from kernel methods, a fruitful direction would be to extend the applicability to more general models using the same paradigm. Scalability is an issue for RKHS-OSV due to matrix inversion but could be alleviated using off the shelf large scale kernel approximation techniques. Finally, it would be interesting to extend our formulation to kernel-based hypothesis testing and for example, to interpret results from two-sample tests.

References

- [Aas et al.(2019)Aas, Jullum, and Løland] Kjersti Aas, Martin Jullum, and Anders Løland. Explaining individual predictions when features are dependent: More accurate approximations to shapley values. *arXiv preprint arXiv:1903.10464*, 2019.
- [Alvarez-Melis and Jaakkola(2018)] David Alvarez-Melis and Tommi S Jaakkola. On the robustness of interpretability methods. *arXiv preprint arXiv:1806.08049*, 2018.
- [Belkin et al.(2006)Belkin, Niyogi, and Sindhwani] Mikhail Belkin, Partha Niyogi, and Vikas Sindhwani. Manifold regularization: A geometric framework for learning from labeled and unlabeled examples. *Journal of machine learning research*, 7(11), 2006.
- [Carvalho et al.(2019)] Diogo V Carvalho, Eduardo M Pereira, and Jaime S Cardoso. Machine learning interpretability: A survey on methods and metrics. *Electronics*, 8(8):832, 2019.
- [Chen et al.(2020)] Hugh Chen, Joseph D Janizek, Scott Lundberg, and Su-In Lee. True to the model or true to the data? *arXiv preprint arXiv:2006.16234*, 2020.
- [Corbett-Davies and Goel(2018)] Sam Corbett-Davies and Sharad Goel. The measure and mismeasure of fairness: A critical review of fair machine learning. *arXiv preprint arXiv:1808.00023*, 2018.
- [Covert et al.(2020)] Ian Covert, Scott Lundberg, and Su-In Lee. Understanding global feature contributions with additive importance measures. *Advances in Neural Information Processing Systems*, 33, 2020.
- [Da Veiga(2021)] Sébastien Da Veiga. Kernel-based anova decomposition and shapley effects—application to global sensitivity analysis. *arXiv preprint arXiv:2101.05487*, 2021.
- [Flaxman et al.(2016)] Seth Flaxman, Dino Sejdinovic, John P Cunningham, and Sarah Filippi. Bayesian learning of kernel embeddings. *arXiv preprint arXiv:1603.02160*, 2016.
- [Frye et al.(2020)] Christopher Frye, Damien de Mijolla, Laurence Cowton, Megan Stanley, and Ilya Feige. Shapley-based explainability on the data manifold. *arXiv preprint arXiv:2006.01272*, 2020.
- [Ghorbani and Zou(2019)] Amirata Ghorbani and James Zou. Data shapley: Equitable valuation of data for machine learning. In *International Conference on Machine Learning*, pages 2242–2251. PMLR, 2019.
- [Hancox-Li(2020)] Leif Hancox-Li. Robustness in machine learning explanations: does it matter? In *Proceedings of the 2020 conference on fairness, accountability, and transparency*, pages 640–647, 2020.
- [Jain et al.(2020)] Aditya Jain, Manish Ravula, and Joydeep Ghosh. Biased models have biased explanations. *arXiv* preprint arXiv:2012.10986, 2020.
- [Janzing et al.(2020)] Dominik Janzing, Lenon Minorics, and Patrick Blöbaum. Feature relevance quantification in explainable ai: A causal problem. In *International Conference on Artificial Intelligence and Statistics*, pages 2907–2916, 2020.
- [Li et al.(2019a)] Z. Li, J.-F. Ton, D. Oglic, and D. Sejdinovic. Towards A Unified Analysis of Random Fourier Features. In *International Conference on Machine Learning (ICML)*, pages PMLR 97:3905–3914, 2019a.
- [Li et al.(2019b)] Zhu Li, Adrian Perez-Suay, Gustau Camps-Valls, and Dino Sejdinovic. Kernel dependence regularizers and gaussian processes with applications to algorithmic fairness. *arXiv preprint arXiv:1911.04322*, 2019.

- [Lundberg and Lee(2017)] Scott M Lundberg and Su-In Lee. A unified approach to interpreting model predictions. In *Advances in neural information processing systems*, pages 4765–4774, 2017.
- [Lundberg et al.(2018)] Scott M Lundberg, Gabriel G Erion, and Su-In Lee. Consistent individualized feature attribution for tree ensembles. *arXiv preprint arXiv:1802.03888*, 2018.
- [Mase et al.(2021)] Masayoshi Mase, Art B Owen, and Benjamin B Seiler. Cohort shapley value for algorithmic fairness. *arXiv preprint arXiv:2105.07168*, 2021.
- [Muandet et al.(2016)] Krikamol Muandet, Kenji Fukumizu, Bharath Sriperumbudur, and Bernhard Schölkopf. Kernel mean embedding of distributions: A review and beyond. *arXiv preprint arXiv:1605.09522*, 2016.
- [Paulsen and Raghupathi(2016)] Vern I Paulsen and Mrinal Raghupathi. *An introduction to the theory of reproducing kernel Hilbert spaces*, volume 152. Cambridge university press, 2016.
- [Pérez-Suay et al.(2017)] Adrián Pérez-Suay, Valero Laparra, Gonzalo Mateo-García, Jordi Muñoz-Marí, Luis Gómez-Chova, and Gustau Camps-Valls. Fair kernel learning. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pages 339–355. Springer, 2017.
- [Rahimi et al.(2007)] Ali Rahimi, Benjamin Recht, et al. Random features for large-scale kernel machines. In *NIPS*, volume 3, page 5. Citeseer, 2007.
- [Ribeiro et al.(2016)] Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. "why should I trust you?": Explaining the predictions of any classifier. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, San Francisco, CA, USA, August 13-17, 2016*, pages 1135–1144, 2016.
- [Schuster et al.(2020)] Ingmar Schuster, Mattes Mollenhauer, Stefan Klus, and Krikamol Muandet. Kernel conditional density operators. In *International Conference on Artificial Intelligence and Statistics*, pages 993–1004. PMLR, 2020.
- [Sejdinovic et al.(2014)] Dino Sejdinovic, Heiko Strathmann, Maria Lomeli Garcia, Christophe Andrieu, and Arthur Gretton. Kernel adaptive metropolis-hastings. In *International conference on machine learning*, pages 1665–1673. PMLR, 2014.
- [Shapley(1953)] Lloyd S Shapley. A value for n-person games. *Contributions to the Theory of Games*, 2(28):307–317, 1953.
- [Shrikumar et al.(2017)] Avanti Shrikumar, Peyton Greenside, and Anshul Kundaje. Learning important features through propagating activation differences. In *International Conference on Machine Learning*, pages 3145–3153. PMLR, 2017.
- [Song et al.(2016)] Eunhye Song, Barry L Nelson, and Jeremy Staum. Shapley effects for global sensitivity analysis: Theory and computation. *SIAM/ASA Journal on Uncertainty Quantification*, 4(1):1060–1083, 2016.
- [Song et al.(2013)] Le Song, Kenji Fukumizu, and Arthur Gretton. Kernel embeddings of conditional distributions: A unified kernel framework for nonparametric inference in graphical models. *IEEE Signal Processing Magazine*, 30 (4):98–111, 2013.
- [Steinwart and Christmann(2008)] Ingo Steinwart and Andreas Christmann. *Support vector machines*. Springer Science & Business Media, 2008.
- [Štrumbelj and Kononenko(2014)] Erik Štrumbelj and Igor Kononenko. Explaining prediction models and individual predictions with feature contributions. *Knowledge and information systems*, 41(3):647–665, 2014.
- [Vapnik(1995)] Vladimir N. Vapnik. The nature of statistical learning theory. Springer-Verlag New York, Inc., 1995.
- [Williams and Rasmussen(2006)] Christopher K Williams and Carl Edward Rasmussen. *Gaussian processes for machine learning*, volume 2. MIT press Cambridge, MA, 2006.
- [Yang et al.(2012)] Tianbao Yang, Yu-Feng Li, Mehrdad Mahdavi, Rong Jin, and Zhi-Hua Zhou. Nyström method vs random fourier features: A theoretical and empirical comparison. *Advances in neural information processing systems*, 25:476–484, 2012.