KernelSHAP-IQ: Weighted Least Square Optimization for Shapley Interactions

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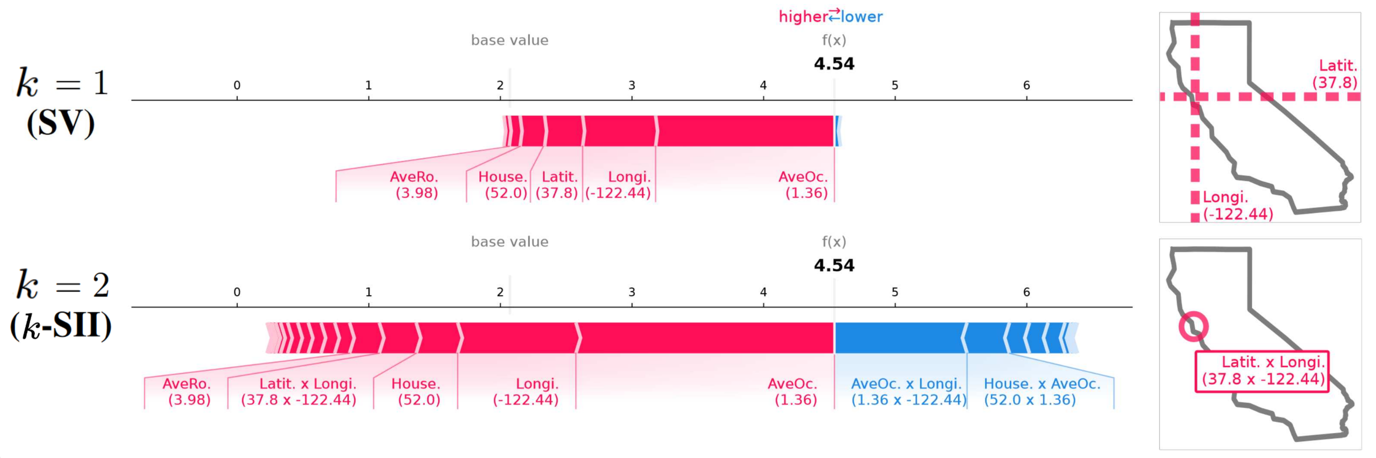
Interaction Example: Explaining Property Prices

Potential Question: "Does the *location* of my property affect its price?"



Background

Shapley Value (SV) [1]:

$$\phi^{SV}(i) = \sum_{T \subseteq N \setminus i} \frac{(n-1-t)! \cdot t!}{n!} \underbrace{[\nu(T \cup i) - \nu(T)]}_{=:\Delta_i(T)}$$

value function (e.g. model prediction)

marginal contribution (increase in collective benefit when i joins T)

Shapley Interaction Index (SII) [2]:

$$\phi^{SII}(S) := \sum_{T \subseteq N \setminus S} \frac{(n-s-t)! \cdot t!}{(n-s+1)!} \underbrace{\sum_{L \subseteq S} (-1)^{s-l} \nu(T \cup L)}_{=:\Delta_S(T)}$$

discrete derivative (synergy effect of S in the presence of T)

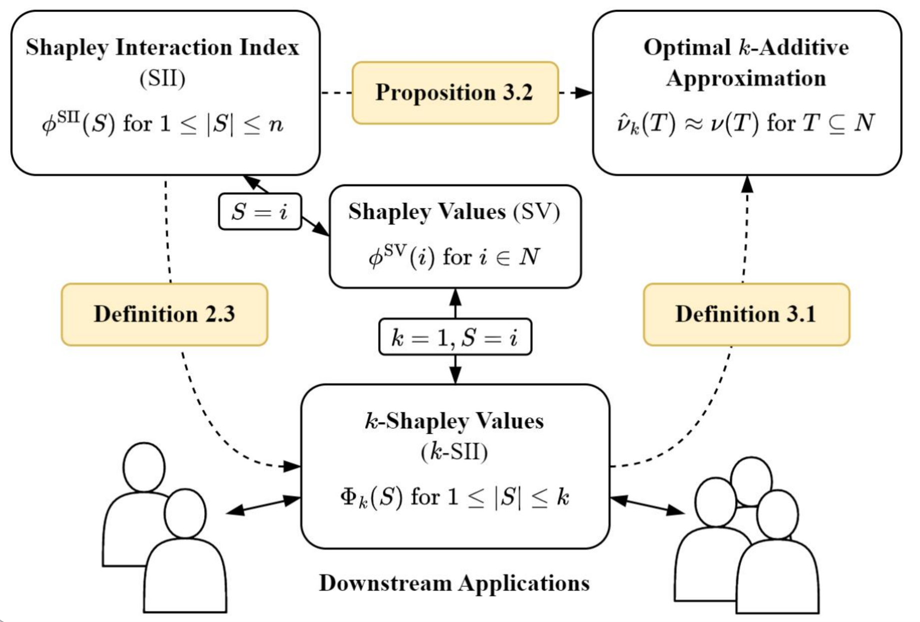
k-Shapley Values (k-SII) [3]:

$$\Phi_k(S) := \begin{cases} \phi^{SII}(S) & \text{if } |S| = k \\ \Phi_{k-1}(S) + B_{k-|S|} \sum_{\tilde{S} \subseteq N \setminus S}^{|S|+\tilde{S}=k} \phi^{SII}(S \cup \tilde{S}) & \text{if } |S| < k \end{cases}$$

Bernoulli numbers

Notation: Player set N; $i,j \in N$; $S \subseteq N$ **Convention:** $s := |S|$ or $n := |N|$

Link between SV, SII and k-SII



Definition 3.1 (k-additive Approximation)

$$\hat{\nu}_k(T) := \sum_{S \subseteq T}^{1 \le |S| \le k} \Phi_k(S)$$

- SII is an order-independent basis index
- k-SII is well-suited for interpretability by adjusting explanation order k

References

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Contribution

TLDR: We present a novel **least-square representation** for the **Shapley Interaction Index** (SII) [2] and present a kernel-based estimator called **KernelSHAP-IQ** akin to KernelSHAP [4] for the Shapley value (SV) [1].

KernelSHAP-IQ

KernelSHAP [4] utilizes a weighted least-square representation:

$$\phi^{SV} = \arg\min_{\phi \in \mathbb{R}^n} \sum_{T \subseteq N}^{0<|T|<n} \mu_1(t) \left[\nu(T) - \sum_{i \in T} \phi(i)\right]^2 \text{ s.t. } \sum_{i \in N} \phi(i) = \nu(N)$$

A new **weighted least-square representation** for the SII:

Theorem 3.7 (KernelSHAP-IQ, $k = 2$). *Let $n \geq 4$ and $(\mathbf{W}_2)_{TT} := \mu_2(t)$. Then the pairwise SII is represented as*

$$\phi_2^{SII} = \lim_{\mu_\infty \to \infty} \arg\min_{\phi_2 \in \mathbb{R}^{\binom{n}{2}}} \left\| \sqrt{\mathbf{W}_2} \, (\mathbf{y}_2 - \mathbf{X}_2 \phi_2) \right\|_2^2.$$

SV residuals; fit for $\hat{\nu}_2$

with:

$$(\mathbf{W}_k)_{TT} := \mu_k(t) := \begin{cases} \binom{n-2 \cdot k}{t-k}^{-1} & \text{if } k \le t \le n-k \\ \mu_\infty & \text{else.} \end{cases}$$

$$(\mathbf{X}_k)_{TS} := \lambda(|S|, |T \cap S|) \text{ for } T, S \subseteq N \text{ with } |S| = k$$

SII-specific weights

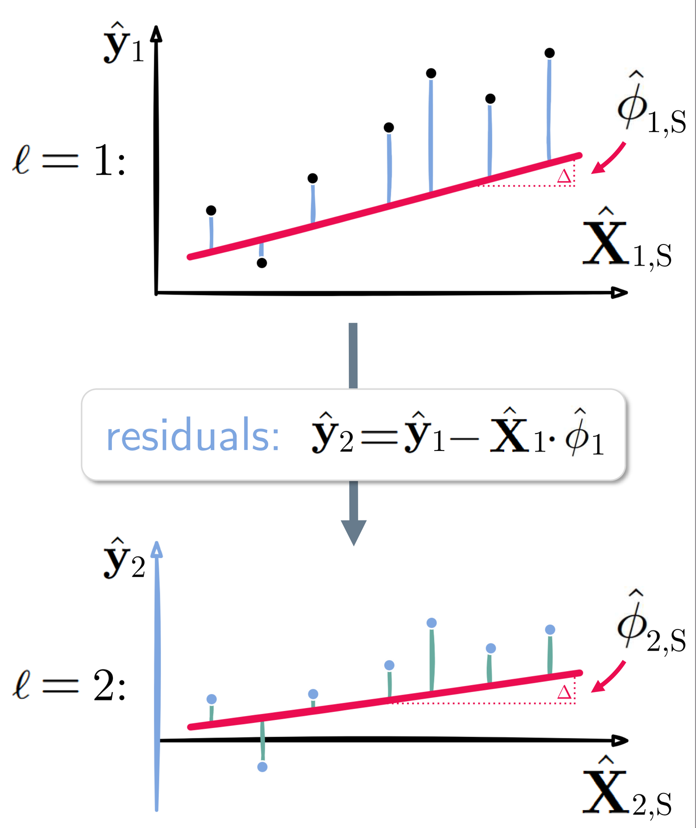
KernelSHAP-IQ is a recursive optimization (simplified for 2-SII):

for order $l = 1, 2$:

- sample subsets from budget $\{T_i\}_i, \{w_T\}_T \leftarrow \textsc{Sample}(b)$
- evaluate game/model $\hat{\mathbf{y}}_1 \leftarrow [\nu(T_1), \ldots, \nu(T_b)]^T$
  - adjust weights per order $\hat{\mathbf{X}}_\ell, \hat{\mathbf{W}}_\ell^* \leftarrow \textsc{Weight}(\ell, \ldots)$
  - solve the regression $\hat{\phi}_\ell \leftarrow \textsc{SolveWLS}(\hat{\mathbf{X}}_\ell, \hat{\mathbf{y}}_\ell, \hat{\mathbf{W}}_\ell^*)$
  - compute residuals $\hat{\mathbf{y}}_{\ell+1} \leftarrow \hat{\mathbf{y}}_\ell - \hat{\mathbf{X}}_\ell \cdot \hat{\phi}_\ell$
- aggregate into k-SII (optional) $\hat{\Phi}_2 \leftarrow \textsc{AggregateSII}(\hat{\phi}_1, \hat{\phi}_2)$

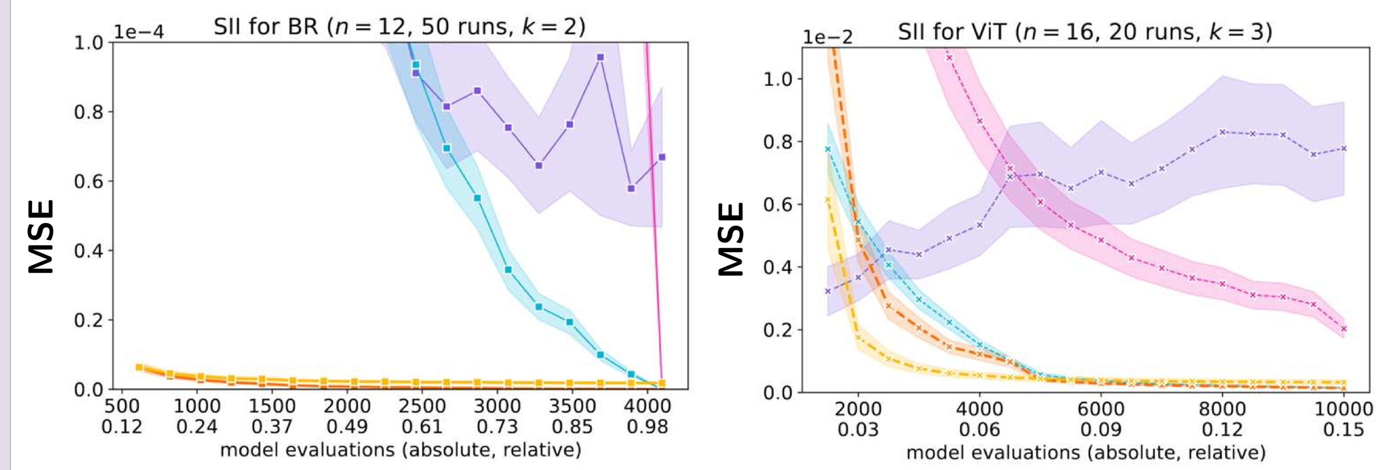
➢ order $l = 1$: KernelSHAP
➢ order $l \geq 2$: KernelSHAP-IQ

illustration for interaction S:

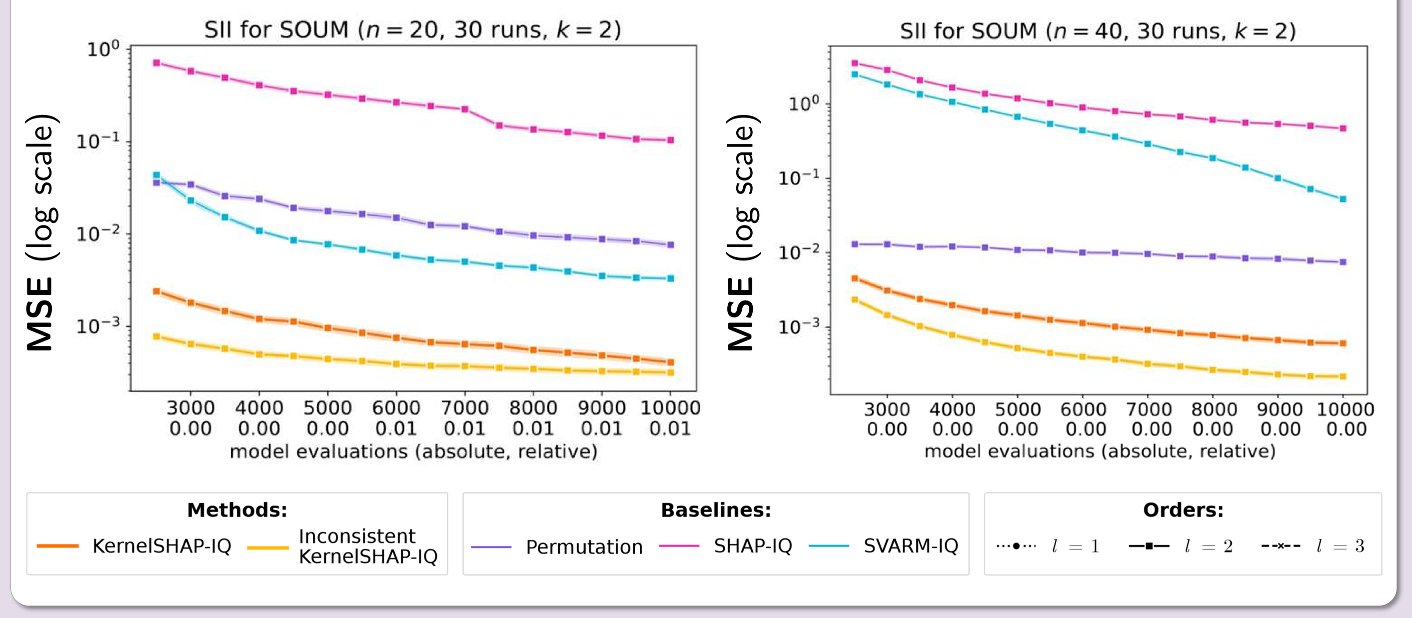


Empirical Results

➢ XAI benchmark for bike regression (BR) and vision transformer (ViT):

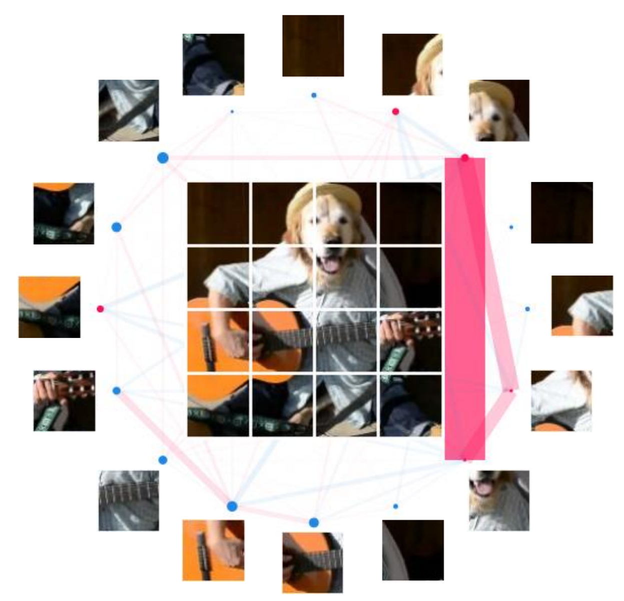


➢ sum of unanimity models (SOUMs) with high number of features n:



Network Plot for a ViT:

- model predicts the class ***golden retriever*** with probability $p_{\max} = 0.203$
- the highest attribution score is the **second order interaction** between the ***head*** and the ***snout***



Open-Source Implementation

- **KernelSHAP-IQ** is available for python

```
pip install shapiq
```

- shapiq includes **18** game theoretic concepts including SV, SII, k-SII, BV, ...
- around **20** approximators and explainers including SHAP-IQ [5], SVARM-IQ [7,9], KernelSHAP [4], k-add SHAP [6], TreeSHAP-IQ [8], ...
- **plot and interpret interactions** with different visualization techniques

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