Fixing Neural Networks by Identifying Top-k Shapley Players

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Abstract

The Shapley value is an important solution concept in cooperative game theory with a variety of applications in the field of Explainable Artificial Intelligence. It is used to provide a fair reward distribution among a given player set representing each player's importance for the respective task. Due to its exponential computational complexity we rely on algorithms approximating the Shapley value given a fixed budget. When applying Shapley values to the structure of a neural network in order to identify neurons responsible for a certain bias for example, we are more interested in the set of the top-k most important players rather than approximating their exact Shapley values. We evaluate algorithms proposed by other authers aswell as introducing our own ideas for the top-k Shapley player problem. Using some of our algorithms we are able to show a relevant difference between the approximation and the top-k problem that allows us to achieve better results than other algorithms that are utilizing their budget similarly efficient. Using another algorithm we were able to identify highly important neurons in a neural network using a budget several magnitudes lower than the current state of the art.

Contents

1 Introduction

Neural networks (NNs), a class of artificial intelligence (AI) models inspired by the human brain, have revolutionized the field of machine learning and data analysis. Their ability to learn from large amounts of data and to make complex predictions is usefull in a variety of different applications, such as image detection, healthcare, text generation and even stock market forecasting [KSH12; Mio+18; Bro+20; Sel+17]. Recently, e.g. large language models, such as OpenAI's GPT models [Bro+20] based on Transformers [Vas+17] are recieving a great amount of attention as they are capable of producing text indistinguishable from human written text and are able to act as a useful assistent in almost every domain. Furthermore, Convolutional Neural Networks (CNNs) have become the state-of-the-art in most image processing applications [LBH15; KSH12]. The size and complexity of modern models increases consistently, with some models containing more than six billion parameters [Bro+20].

However, NNs can often appear as black boxes to the human eye, with little to no transparency about their inner mechanisms as the interactions between neurons can seem arbitrary and are hard to track. Even though the mathematics for evaluating a single neurons are rather simple, the enormous number of neurons and connections make it very difficult to comprehend an outcome of the model. Therefore, even though NNs achieve far better results than their specialized competitors in many applications, explaining their decisions poses a quite challenging task. A bank for example might use a NN to decide whether a client recieves a credit based on properties such as income, age, and profession. If the credit gets declined, the bank is required to explain why this decision was made, which is challenging in the case of a NN. A Neural Network's precision and verstility immensely depend on the training data it recieves. Similar to a child growing up in a household with abusive or careless parents and adapting their behaviour over time, a NN trained on biased data will most likely output biased predictions aswell. Therefore, it is really important to chose the training data carefully. However, as more sophisticated machine learning models emerge, they often demand an increasing amount of data for effective training. Otherwise, models with a large amount of parameters tend to overfit to the training data, basically memorizing each prediction. This phenomenon

has a bad impact on the versatility of a model.
GPT-3 for example, is trained on a dataset consiting of about 500 billion tokens [Bro+20], where ach token represents roughly half a word. For such huge datasets it is practically infeasable to examine all of it. As a result, quantity often outweighs quality in practical applications.
Howard et al. [HB18] present a variety of real examples of biased AI models. In 2015 for example, Google released a face recognition application that mislabeled black people as "gorillas". A reason for that might have been the training data origing from mostly european countries where people of color are underrepresented. Biases in the real world against minorities for example are often transfered directly to the internet. Large language models, such as OpenAI's GPT models [Bro+20], often suffer from this problem as they are directly trained on large chunks of data available on the internet. Brown et al. [Bro+20] state themselves that GPT-3 has certain biases in gender, race and religion. Popular prejudices about the Islam for example are adopted by GPT-3 with words like "violent", "terrorism" and "terrorist" occuring more often with Islam than with other religions.
Even though we are able to observe such biases, discovering how they are created is practically infeasable from inspecting the network architecture with just the human eye. This problem incentivizes research on methods that make the black box problem more transparent.

The field of *Explainable Artificial Intelligence* (XAI) aims to understand and address such behaviors. The Shapley value [Sha+53], a solution concept from cooperative game theory, is a useful tool for identifying biases in ML models. Many XAI problems can be reformulated as so called cooperative games. In these games players form arbitrary coalitions to achieve a collective benefit. The Shapley value of a player represent its importance for the respective game. Shapley's [Sha+53] solution doesn't require any knowledge about how the value of a coalition is calculated which is ideal for ML models. Intuitively this works by adding and removing a player from a coalition and inspecting the change in worth. The worth of all players combined is then distributed among all players according to their average contribution to any coalition. For measuring local feature importance, i.e. the importance of each feature for a single prediction, the input features of a model are treated as players [Roz+22] and coalitions are evaluated by running the model with subsets of features. For example, in the case of declined credit, the Shapley values of the client's properties could be calculated to determine which ones had the most impact on the decision. This way, a previous gambling addiction, for example, could be identified as the main cause of the rejection. In addition, when looking at global feature importance it is possible to determine how much weight a model gives to a

feature in general by computing Shapley values using the whole dataset [Mol20]. This might be interesting to verifiy if a client's income is the main aspect for a credit algorithm's decision.

Ghorbani et al. [GZ20] propose treating the neurons of a NN as players where the worth of a coalition of players is represented by the network's accuracy when only a subset of neurons are used. This approach allows for ranking the importance of all the neural network's neurons by their Shapley values. Neurons with a negative Shapley value would predominantly contribute negatively to the model's performance and could be completely removed. Another use case is when a model's bias is known. By evaluating the Shapley values on a specialized dataset, the neurons responsible for this bias can be identified and eliminated. Ghorbani et al. [GZ20] demonstrate that this method significantly reduces a model's bias.

In practice we are unable to calculate the exact Shapley value in most usecases, as the number of coalitions that have to be evaluated scales exponentially with the number of players. Therefore we rely on algorithms that approximate the value with as little evaluated coalitions as possible [CGT09; KBH23]. For many applications such as determining neuron importance, it is sufficient to find the top-k players with the highest Shapley values as defined by Kolpaczki et al. [KBH21]. This problem statement has fewer requirements compared to the approximation of the Shapley value for all players. Ghorbani et al. [GZ20] employed a top-k algorithm to identify the most important neurons in a neural network.
The aim of this thesis is to evaluate existing top-k and approximation algorithms on the top-k problem and to discover additional top-k Shapley player algorithms with the aim of applying them in XAI tasks similar to the work of Ghorbani et al. [GZ20]. With our algorithms HybridApproBUS and HalfBUS we are able to achieve partially better results than established algorithms and discover that updating all playeres using similar coalition values is a meaningfull concept for the top-k problem as it makes the approximated Shapley values of the players more comparable. Using a variant of Kolpaczki et al.'s work [KBH23] we are able to achieve part of Ghorbani et al.'s results [GZ20] in a significantly more efficient way.

2 Fundamentals

2.1 Cooperative Games

The cooperative game is a concept from game theory where players form arbitrary groups, so called coalitions, to achieve a collective reward.

Definition 2.1.1 (Cooperative game)**.** Given a player set $N = \{1, ..., n\}$ with $n \in \mathbb{N}$ and a value function $v : \mathcal{P}(N) \to \mathbb{R}$ with $v(\emptyset) = 0$, the tuple (N, v) denotes a n-player cooperative game.

The coalition formed by all players is often refered to as the grand coalition. Let's consider the scenario of a class of 20 students that are working jointly in a project. They can form arbitrary groups to complete this task. Each student represents a player and the value function is the grade or the number of credits a group of students would recieve for their project.

2.2 The Shapley Value

Looking at the classroom setting, students have to be graded seperatly as it is common for some students ~~to~~ contribute more to the task than others which would make grading all students equally unfair.
In cooperative games the challenge is to find a fair distribution $(\phi_i)_{i \in N}$ of real values that assigns a numerical payoff to each player i representing their importance to the game without knowing how the value function is calculated. I.e. in our classroom the teacher would have to assess to outcome of the project without monitoring the progress of the group.
The Shapley value is a solution concept for each player's payoff in a cooperative game [Sha+53].

Definition 2.2.1 (Shapley value)**.** Given a cooperative game (N, v) the Shapley value of a player $i \in N$ is defined as:

$$\phi_i = \sum_{S \subseteq N \setminus \{i\}} \frac{1}{n\binom{n-1}{|S|}} [v(S \cup \{i\}) - v(S)]. \tag{2.1}$$

Intuitively, it represents a player's average marginal contribution. The marginal contribution $v(S \cup \{i\}) - v(S)$ of a player i is the difference in worth of a coalition S that doesn't contain the player compared to when the player is added.

The Shapley value is provably the only solution that garantees a certain set of axioms which arguably capture fairness [KBH23]. These four axioms are:

- Efficiency: The worth of the grand coalition, the coalition that is formed by all players combined is shared among all players:

$$\sum_{i \in N} \phi_i = v(N).$$

- Symmetry: The payoff of two players $i, j \in N$ should be the same if they contribute equally to every coalition:

$$(\forall S \subseteq N \setminus \{i, j\} : v(S \cup \{i\}) = v(S \cup \{j\})) \implies \phi_i = \phi_j.$$

- Dummy player: A player $i \in N$ that does not contribute to any coalition has a payoff of zero:

$$(\forall S \subseteq N \setminus \{i\} : v(S \cup \{i\}) = v(S)) \implies \phi_i = 0.$$

- Additivity: If the cooperative game can be split up into subgames, i.e. $v = v_1 + v_2$ with $v, v_1, v_2 : \mathcal{P}(N) \to \mathbb{R}$, the payoff of each player i in the combined game should be the sum of its payoff in the respective subgames:

$$\phi_i^v = \phi_i^{v_1} + \phi_i^{v_2}.$$

A very basic example of a cooperative game would be a game where each coalition $S \subseteq N = \{1, ..., n\}$ recieves its length as its value i.e. $v(S) = |S|$. Finding the

Shapley values for this game is a trivial task as each player contributes equally to the length of the coalition. As a consequence $\phi_i = \frac{1}{v(N)} = \frac{1}{n}$ for all $i \in N$. Cooperative games that are formulated in such a way that the Shapley values are immediately apparent or can be calculated in polynomial time are called synthetic cooperative games.

However, this is not the case for most applications. In fact, from eq. (2.1) it is easy to see that in general in order to calculate the Shapley value for all n players the value function would have to be evaluated for every subset of N resulting in $|\mathcal{P}(N)| = 2^n$ calculations making it an NP-hard problem [KBH23]. This poses an inevitable burden to the application of the Shapley value in XAI. Consider an image detection algorithm, identifying 32×32 pixel images. In order to determine which details of the image the algorithm focused on, one could use the loss function of the model as a value function and consider each pixel as a player and calculate the respective Shapley values. For 32×32 pixel images this would be 1024 players with $2^{1024} \approx 10^{308}$ possible coalitions. The model would have to be run and the loss function calculated for each of these coalitions. Obviously, this is a practically infeasible task.

Because of this drawback, we have to rely on algorithms approximating the Shapley value. In order to approximate a large sum as in eq. (2.1) one can treat the set of all coalitions as possible realizations of a random variable with the respective marginal contributions as values and approximate the expected value of that random variable. Given a player $i \in N$, let X denote a random variable with values $(x_S)_{S \subseteq N \setminus \{i\}}$ where $x_S = v(S \cup \{i\}) - v(S)$ and probability distribution $P(S) = \frac{1}{n\binom{n-1}{|S|}}$. Then the expected value of X exactly matches the player's Shapley value, i.e.:

$$E[X] = \sum_{S \subseteq N \setminus \{i\}} x_S \cdot P(S) = \phi_i \tag{2.2}$$

~~holds true.~~ Therefore in order to approximate the Shapley value of a player i we can approximate the expected value of X instead. For a total of m samples $(S_j)_{j \in \{1,\dots,m\}}$ with each $S_j \subseteq N \setminus \{i\}$ we get an estimator for our Shapley value:

$$\hat{\phi}_i = \frac{1}{m} \sum_{j=1}^{m} x_{S_j}. \tag{2.3}$$

Approximation algorithms are mostly based on this concept of sampling coalitions but often use a transformed version of eq. (2.1) in order to optimize the sampling process and optain an accurate estimator while calling the value function as little as possible.

2.3 Problem of Identifying Top-k Shapley Players

For some applications it is not necessary to get reasonably precise approximations for every player. It might be interesting enough to know which players are the most important. For example, when trying to reduce the size of a neural network one would want to know the k most important neurons in order to retain them while dropping the rest [GZ20]. Kolpaczki et al. [KBH21] define the Top-k Shapley problem:

Definition 2.3.1 (Top-k Shapley problem)**.** Given a cooperative game (N, v) and $k \in N$ find a set $K := \{i \in N \mid \phi_i \geq \phi_{\pi(k)}\}$ for a permutation $\pi \colon N \to N$ such that $\phi_{\pi(1)} \geq \ldots \geq \phi_{\pi(n)}$.

K contains the Players with the k highest Shapley values.
With this formulation of the problem the exact Shapley values of the players become less important. This allows for a lot more optimization as the sampling procedure can shift the focus to a smaller subset of players that are highly uncertain to be part of the top-k players while players with very high or very low Shapley values can be classified rather quickly [KBH21].
Like Kolpaczki et al. [KBH21] we focus on a fixed budget scenario where the performance of an algorithm is measured by its ability to identify the top-k players given a budget $T \in \mathbb{N}$. T is the number of times the algorithm is allowed to call the value function as in most applications the value function is the bottleneck. In XAI tasks for example the value function often includes an evaluation of the AI model which is usually quite expensive to compute.

In addition we need to establish metrics that measure an algorithm's performance. Using synthetic cooperative games that allow us to calculate the exact Shapley values in polynomial time we can compare the algorithm's estimation with the actual value.

For approximation algorithms a common performance metric is the *mean squared error* (MSE) where the the squared differences between the approximation and the actual Shapley values of all players are averaged:

$$MSE = \frac{1}{n} \sum_{i \in N} (\phi_i - \hat{\phi}_i)^2.$$

However, this metric does not provide any information on the performance on the top-k problem because an algorithm does not need to approximate all Shapley values precisely but find the players with the highest values. In theory an algorithm does not need to return the approximated Shapley values. But since all of our algorithms internally work with approximations of the values we keep the MSE to compare an algorithm's performance on the top-k problem and the approximation problem.

We define the following performance metric for the top-k problem. Using a permutation $\pi : N \to N$ such that $\phi_{\pi(1)} \geq ... \geq \phi_{\pi(n)}$, $K := \{i \in N \mid \phi_i \geq \phi_{\pi(k)}\}$ denotes the set of players with the k highest Shapley values. We propose two measures:

$$\psi(\hat{K}) = \begin{cases} 1, & \text{if } \hat{K} \subseteq K \\ 0, & \text{otherwise} \end{cases} \tag{2.4}$$

$$\varphi(\hat{K}) = \frac{|\hat{K} \cap K|}{|\hat{K}|} \tag{2.5}$$

Equations (2.4) and (2.5) formulate a nominal scale ψ and a ratio scale φ for an algorithm's estimation $\hat{K}$ of the top-k players with $|\hat{K}| = k$. Similar to Kolpaczki et al.'s evaluation [KBH21] ψ returns one if the algorithm delivered a valid set of k players and zero if it didn't. φ returns the ratio of players that the algorithm correctly classified as part of the top-k players.
For most of our evaluations we use the ratio scale as it has a continuous range of values, making it easier to differenciate multiple results.

Example 2.3.1 (The Advantage of the ratio scale). Let $K = \{1, 2, 3, 4\}$. Suppose we have two algorithms approximating K with results $\hat{K}_1 = \{1, 2, 3, 5\}$ and $\hat{K}_2 = \{5, 6, 7, 8\}$. Intuitivly, the result of algorithm 1 is better than the result of algorithm 2 as it has found most of the top-k players. However, the performance of both algorithms would be measured equal using the nominal scale $\psi(\hat{K}_1) = \psi(\hat{K}_2) = 0$ as they both haven't found the correct set. The ratio scale differenciates between the results returning $\varphi(\hat{K}_1) = 3/4$ for algorithm 1 and $\varphi(\hat{K}_2) = 0$ for algorithm 2.

In addition to calculating the performance metric of an algorithm we have to run the experiment multiple times and average the results over all experiments since the sampling process in most algorithms is randomized and won't always deliver the same result. In order to determine if we conducted enough experiments we calculate the standard error of our averaged result which estimates how confident

the result is. Given a vector of $m \in \mathbb{N}$ results $(x_i)_{i=1}^m$, the sample variance [@Wei03] of the algorithm's performance is calculated using

$$\hat{\sigma}^2 = \frac{1}{m-1} \sum_{i=1}^{m} (x_i - \bar{x})^2,$$

where $\bar{x} = \frac{1}{m} \sum_{i=1}^{m} x_i$ is the average result. In case of the ratio scale we use $x_i = \varphi(K_i)$. The standard error (SE) is then calulated using

$$SE = \frac{\hat{\sigma}}{\sqrt{m}}.$$

2.4 Neural Networks

In the following section we'll give a short explaination of Neural networks (NNs) and how they work. A more in depth explaination can be found in Charu C. Aggarwal's *Neural Networks and Deep Learning: A Textbook* [Agg+18].

Neural Networks are machine learning models are designed to work similar to the human brain in order to accomplish tasks that are to complex to be explicitly programmed using traditional rule-based methods. Instead a NN learns patterns and relationships within data through a training process.
Modern NNs achieve astonishing results: Brown et al's language model GPT-3 [Bro+20] in its largest version is able to produce news articles nearly indistinguishable from articles written by humans as the accuracy of humans classifying these aticles is close to chance. Image generation models, such as stable diffusion [@AI22] and DALL-E 2 [Ram+22], are capable of producing realisitc images from simple text prompts as shown in fig. 2.1.

A NN is structured into layers of nodes, called neurons, a reference to the human brain. Each neuron takes input signals, performs a computation, and produces an output signal that is passed on to the next layer.
The first layer of the network, the input layer, receives the initial data. This data could be anything, ranging from text or sound waves up to image data, as long as it can be serialized into a vector of real numbers. The last layer is the output layer, which produces the final prediction or output of the network. Between these two layers, there can be one or more hidden layers, which extract and transform features from the input data.

(a) a propaganda poster depicting a cat dressed as french emperor napoleon holding a piece of cheese

(b) a teddy bear on a skateboard in times square

Fig. 2.1: Samples generated by DALL-E 2 [Ram+22] and the corresponding prompts

Figure 2.2 illustrates the structure of a neural network. Each connection between neurons is assigned a weight w_i. A neuron recieves the output of all d neurons of the previous layer $(x_i)_{i=1}^d$ in order to produce its output. Different types of NNs or rather NN layers perform different types of operations on its input. CNNs for example pass data through multiple layers of so called filters in order to identify certain patterns, in images mainly. In a simple linear layer however, the output of a neuron is a linear combination of its inputs and its weights summed with an invariant bias b:

$$\sum_{i=1}^{d} w_i x_i + b.$$

An activation function, such as the sign function:

$$sign(x) = \begin{cases} -1 & \text{if } x < 0, \\ 0 & \text{if } x = 0, \\ 1 & \text{if } x > 0 \end{cases}$$

is applied to the output of a layer in order to achieve non-linear results. This is particularly usefull for classification tasks where the data is not linearly seperable into two classes [Agg+18].

NNs learn by adjusting the weights of connections between neurons. During training, the network is presented with input data along with the correct outputs. The output

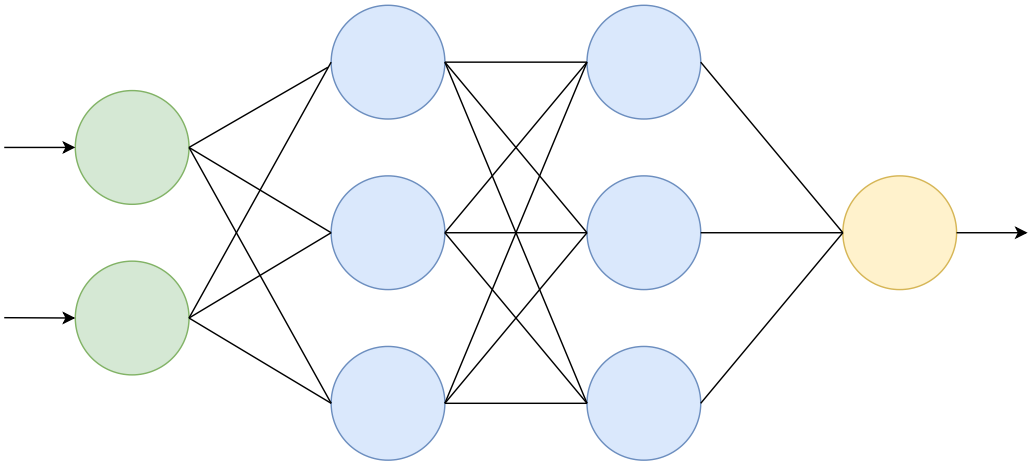


Fig. 2.2: Simplified illustration of a neural network: input layer (green), hidden layers (blue), output layer (yellow)

of the NN for a single data point based on the current weights is compared to the true label, measuring the loss. The weights are then updated using an optimization algorithm, such as gradient descent, that tries to minimize the the loss.

2.4.1 Feature Importance

Going back to the "black box" problem of neural networks we can use Shapley values to calculate the importance of input features for a machine learning model both for a single prediction or for the whole dataset [Mol20]. This can help understand what the major reasons for the model's decision are. For image detection models for example, this enables us to identify the areas of the image that were most influencial for the algorithm [LL17]. When applying Shapley values on feature importance the input features form the set of players and the performance of the model is used as the value function. Of course, in order to calculate the value function for subsets of the player set we need to remove input features. Simply removing the input neuron of this feature, which yields the same result as fixing its output to zero, would negatively influence the model since zero itself could already carry some information. In the image detection example this would be a black pixel. Depending on the image, setting a pixel to zero could completely change the image (if it is mostly light) or not change the image at all (if it is mostly dark). To address this, removed features are most often replaced by their average or a random value.

2.4.2 Neuron Shapley

Large ML models can be incredibly time-consuming to train and require an extensive amount of training data. Therefor, when biases are detected, the process of cleaning the training data and retraining the model can become impractical. It would be ideal if we could identify and eliminate specific neurons in the model that we consider responsible for these biases. To address this, Ghorbani et al. [GZ20] introduced the concept of *Neuron Shapley*.
Out of the NN and the available data a cooperative game can be constructed, where each neuron represents a player. A performance metric, such as accuracy, is used as the value function v. For image classifications tasks the accuracy of a model is the ratio of correctly labeled image from a sampled batch.
To run the model using only a subset of neurons, the remaining neurons need to be deactivated. However, simply replacing the output of these neurons with zeros would negatively impact the mean statistic of the corresponding layer, which would in turn affect other neurons (similar to removing features in section 2.4.1). Therefore, instead of replacing the output with zeros, Ghorbani et al. [GZ20] propose replacing the output of deactivated neurons with their mean output. This approach ensures that the subsequent neurons still receive inputs that are not completely new values.

Ghorbani et al. [GZ20] employ their method on the Inception-v3 [Sze+16] CNN model, consisting of 17216 filters that are used as players and are able to identify the most important filters of each layer. By inspecting these filters' strongest activations they are able to explain the main workflow of the model. Early layers tend to detect general concepts of images such as main colors or shapes while deeper layers tend to be more task specific detecting e.g. animal eyes as shown in fig. 2.3.

In addition, they are able to target class specific neurons by calculating Shapley values on certain image classes. For Zebras, a filter activated by images containing stripes is critical while a filter activated by crowded objects is important to detect Carousels. They also show that they can strongly reduce the models accuracy in specific classes by removing up to 40 important neurons while retaining most of the models' overall accuracy. A similar method is also used to reduce biases towards certain demographics in a SqueezeNet [Ian+16] model trained to detect gender from faces.

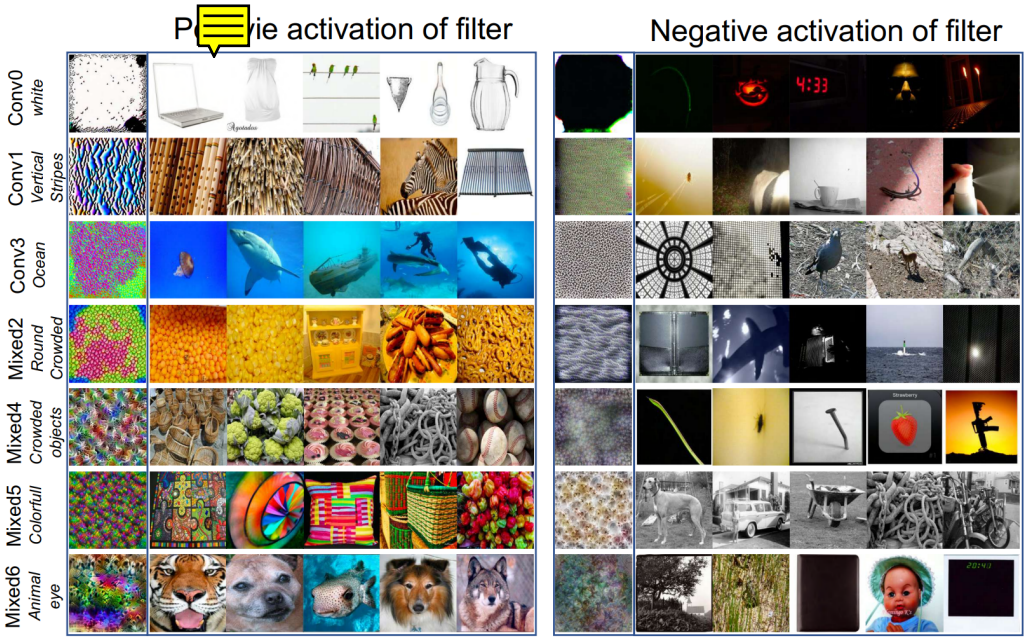


Fig. 2.3: Ghorbani et al.'s [GZ20] visualization of filters with highest Shapley values for a selection of Inception-v3 layers. For each filter, 5 images with most positve or negative activation of the respective neuron are displayed giving the filter a meaningful interpretation. On the left they provide an image that is optimized to strongly activate the filter.

3 Algorithms

In this thesis, we aim to conduct a comprehensive comparison of algorithms on the Top-k Shapley problem. Our primary focus is on evaluating the core algorithms in order to discover which concepts work the best for the challenge at hand, avoiding any bias towards specific use cases. Furthermore, each algorithm is modified to keep the Shapley value estimator $\hat{\phi}_i$ of each player $i \in N$ up to date. The algorithms are formulated to run indefinitely but are stopped when the budget is depleted and the top-k players can be inferred by sorting the estimated values. Modifications and added details are marked in color.

All the algorithms under evaluation operate by evaluating the value funtion for sampled coalitions and utilizing the obtained coalition worth to update the estimated Shapley values of certain players. No matter the coalition, for every player exactly one other coalition exists such that the two coalitions can be used to compute a marginal contribution of that player. Therefore, in theory each sampled coalition's worth could be used to update all players Shapley values if the value of the matching coalition for the player is known. To quantify the effectiveness of an algorithm in updating its Shapley values, we introduce the concept of *budget efficiency*.

Definition 3.0.1 (Budget efficiency)**.** For a cooperative game (N, v), the budget efficiency β of an algorithm is defined as the ratio between the number of marginal contributions used to update the Shapley value estimate of any player $i \in N$ and the consumed budget (number of value function evaluations).

Example 3.0.1 (Perfect Budget efficiency). Consider an algorithm that calculates the worth $v(S)$ of all 2^n coalition $S \subseteq N$ once and uses these values to calculate the Shapley values of all players. As each Shapley value represents the weighted average of 2^{n-1} marginal contributions, this approach yields a budget efficiency of $\beta = \frac{n2^{n-1}}{2^n} = \frac{n}{2}$.

Example 3.0.2 (Budget efficiency of a simple approximation algorithm). A very basic approximation algorithm would iterate through the players $i = 1, ..., n$, sample

coalitions $S \subseteq N \setminus \{i\}$ with probability distribution $P(S) = \frac{1}{n\binom{n-1}{|S|}}$ and compute the marginal contribution $v(S \cup \{i\}) - v(S)$ in order to improve the players Shapley value estimator, according to eq. (2.3). Each marginal contribution update requires two value function evaluations, resulting in a budget efficiency of $\beta = \frac{1}{2}$.

In the following sections we present a selection of algorithms proposed in the literature, the core ideas behind them and our modifications. In addition we introduce our own algorithms for the top-k Shapley problem.

3.1 ApproShapley

Castro et al. [CGT09] proposed a simple yet powerful approximation algorithm called *ApproShapley*. This algorithm is based on the idea of sampling permutaions $O : N \to N$ of the player set $N = \{1, ..., n\}$ instead of sampling coalitions directly. $\pi(N)$ denotes the set of all $n!$ possible permutations. For simplicity, we often define a permutation $O \in \pi(N)$ as a vector $O = (O(1), ..., O(n))$ of players. Using this notation a permutation is interpreted as an ordering of the players where $O(j) = i$ implies that player i is at the jth position in the sequence. Castro et al. [CGT09] approximate the Shapley value using an equation equivalent to eq. (2.1):

$$\phi_i = \sum_{O \in \pi(N)} \frac{1}{n!} [v(Pre^i(O) \cup \{i\}) - v(Pre^i(O))], \tag{3.1}$$

where $Pre^i(O) = \{O(1), ..., O(k-1)\}$ is the predecessor set of player i in a permutation $O \in \pi(N)$, with $i = O(k)$. The algorithm functions by uniformly sampling a random permutation with probability $\frac{1}{n!}$ in each iteration. The sampled permutation O is then used to compute a marginal contribution for each player. This is achieved by iterating through the permutation and updating the current player i using the values of the predecessor set $Pre^i(O)$ with and without the player added.
Although the paper does not explicitly demonstrate it, ApproShapley can be optimized to utilize only one value function call per update. This optimization is possible because the value of the predecessor set combined with the current player $O(k)$ can be reused to calculate the marginal contribution of the next player $O(k+1)$, since $Pre^{O(k)}(O) \cup \{O(k)\} = Pre^{O(k+1)}(O)$.

Example 3.1.1. Consider a player set $N = \{1, 2, 3\}$, and assume we sample the permutation $(2, 3, 1)$. The respective marginal contributions are calculated as follows:

1. Player 2:
$$v(Pre^2((2,3,1)) \cup \{2\}) - v(Pre^2((2,3,1)))$$
$$= v(\{2\}) - v(\emptyset)$$

2. Player 3:
$$v(Pre^3((2,3,1)) \cup \{3\}) - v(Pre^3((2,3,1)))$$
$$= v(\{2,3\}) - v(\{2\})$$

3. Player 1:
$$v(Pre^1((2,3,1)) \cup \{1\}) - v(Pre^1((2,3,1)))$$
$$= v(\{2,3,1\}) - v(\{2,3\})$$

With this approach, we can reuse the values for each player except for the values of the empty set, which is always zero, and the grand coalition. Consequently, updating every player once requires only $n = 3$ value function calls.

Due to this behavior, ApproShapley (Algorithm 1) achieves a budget efficiency of $\beta = \frac{n}{n} = 1$.

Algorithm 1 optimized ApproShapley

Require: $(N = \{1, .., n\}, v)$
  $\hat{\phi}_i \leftarrow 0, t_i \leftarrow 0$, for all $i \in N$
  while $true$ **do**
    Sample $O \in \pi(N)$ uniformly with probability $\frac{1}{n!}$
    $pre \leftarrow 0$
    for $i \in N$ **do**
      $p \leftarrow O(i)$
      $t_p \leftarrow t_p + 1$
      $\delta_{p,t_p} \leftarrow v(Pre^p(O) \cup \{p\}) - pre$
      $\hat{\phi}_p \leftarrow \frac{(t_p - 1)\hat{\phi}_p + \delta_{p,t_p}}{t_p}$
      $pre \leftarrow \phi_{p,t_p} + pre$
    end for
  end while

3.2 SVARM and Stratified SVARM

When inspecting eq. (2.1), we can observe that for each player i, the value $v(S)$ of every coalition $S \subseteq N$ will be added to the sum if $i \in S$, or subtracted if $i \notin S$. Kolpaczki et al. [KBH23] propose an approach to efficiently update multiple players' marginal contributions simultaneously by approximating two separate sums by transforming eq. (2.1) to:

$$\phi_i = \sum_{S^+ \subseteq N \setminus \{i\}} \frac{v(S^+ \cup \{i\})}{n\binom{n-1}{|S|}} - \sum_{S^- \subseteq N \setminus \{i\}} \frac{v(S^-)}{n\binom{n-1}{|S|}}. \tag{3.2}$$

When sampling a coalition though, we have to keep in mind that two coalitions forming a marginal contribution have different sizes. Kolpaczki et al. [KBH23] demonstrate that to avoid introducing a bias, the probability distributions for sampled coalitions S^+ (used for positive updates) and S^- (used for negative updates) need to satisfy the following condition for all $i \in N$ and $S \subseteq N \setminus \{i\}$:

$$P(S^+ = S \cup \{i\} \mid i \in S^+) = P(S^- = S \mid i \notin S^-) = \frac{1}{n\binom{n-1}{|S|}}.$$

By using seperate distributions for S^+ and S^- that satisfy this condition, the authors introduce the algorithm *Shapley Value Approximation without Requesting Marginals* (SVARM)[KBH23], which updates the positive sum for all players $i \in S^+$ and the negative sum for all players $i \in S^-$ by sampling coalitions S^+ and S^- in alternating fashion and evaluating $v(S^+)$ and $v(S^-)$ respectively.

Kolpaczki et al. [KBH23] further enhance SVARM, eliminating the need for seperate probability distributions, by employing stratification: The Shapley value's sum is rearranged into multiple sums that can be approximated seperately with each one summing over all coalitions of a specific length. Equation (2.1) is reformulated as:

$$\phi_i = \frac{1}{n} \sum_{l=0}^{n-1} \phi_{i,l}^+ - \phi_{i,l}^-, \tag{3.3}$$

with:

$$\phi_{i,l}^+ = \sum_{S \subseteq N \setminus \{i\}, |S|=l} \frac{v(S \cup \{i\})}{\binom{n-1}{l}} \tag{3.4}$$

$$\phi_{i,l}^- = \sum_{S \subseteq N \setminus \{i\}, |S|=l} \frac{v(S)}{\binom{n-1}{l}}. \tag{3.5}$$

The stratas $\phi^+_{i,l}$ and $\phi^-_{i,l}$ can be approximated in a similar fashion as $\hat{\phi}_i$ in eq. 2.3. Kolpaczki et al.'s *Stratified SVARM* (StratSVARM) [KBH23] functions by sampling a coalition $S \subseteq N$ and calculating $v(S)$. For every player i, it updates $\hat{\phi}^+_{i,|S|-1}$ if $i \in S$ and $\hat{\phi}^-_{i,|S|}$ if $i \notin S$. This enables an update of every player's Shapley value with each call of the value function. As in theory each sampled coalition resembles half of a marginal contribution StratSVARM has a budget efficiency of $\beta = \frac{n/2}{1} = \frac{n}{2}$ basically the best possible budget efficiency, regarding example 3.0.1.

Remark 3.2.1. It is important to note that StratSVARM doesn't directly update marginal contributions. Updating $\hat{\phi}^+_{i,l}$ and $\hat{\phi}^-_{i,l}$ once each, using samples $S_1, S_2 \subseteq N$, might not be as valuable as updating $\hat{\phi}_i$ using a complete marginal contribution $v(S \cup \{i\}) - v(S)$.

The sampling strategy for the length of a coalition is arbitrary. Each $\hat{\phi}^+_{i,l}$ and $\hat{\phi}^-_{i,l}$ is approximated separately, enabling Kolpaczki et al. [KBH23] to choose a probability distribution with desirable mathematical properties for l.
We remove the algorithm's warmup phase as it requires a substantial amount of budget and is needed mostly for theoretical guarantees.

In addition to StratSVARM we propose *Truncated Stratified SVARM* (algorithm 2) for Neuron Shapley applications. This simplified version of StratSVARM includes the feature of truncation. With enough neurons removed, the accuracy of most neural networks drops to zero. Consequently $\phi^+_{i,l}$, $\phi^-_{i,l} \approx 0$ for $l < \delta$ with a certain size threshold $0 \leq \delta < n$ which makes TruncStratSVARM even more memory efficient. We can abstain from evaluating coalitions smaller than δ and sample l uniformly at random from the remaining sizes. Like Stratified SVARM, TruncStratSVARM updates all $\hat{\phi}^+_{i,l-1}$ for $i \in S$ and $\hat{\phi}^-_{i,l}$ for $i \notin S$ using a uniformly sampled coalition $S \subseteq N$ with $|S| = l$. Additionally, the exact calculation of StratSVARM, which involves computing stratas of certain sizes exactly, is minimized since calculating the the value for all coalitions of size 1 and $n-1$ would require $2n$ value function calls which is a substantial portion of the budget we have available in our evaluation. Also $1 \ll \delta$ most of the time.

Algorithm 2 TruncStratSVARM

Require: cooperative game $(N = \{1, .., n\}, v)$, $0 \leq \delta < n$
  $\hat{\phi}^+_{i,l}, \hat{\phi}^-_{i,l} \leftarrow 0$, for all $i \in N, l \in \{\delta, ..., n-1\}$
  $c^+_{i,l}, c^-_{i,l} \leftarrow 0$, for all $i \in N, l \in \{\delta, ..., n-1\}$
  $\hat{\phi}_i \leftarrow 0$, for all $i \in N$
  $\hat{\phi}^+_{i,n-1} \leftarrow v(N), c^+_{i,n-1} \leftarrow 1$, for all $i \in N$
  while $true$ **do**
    Draw $l \in \{\delta + 1, ..., n-1\}$ uniformly at random
    Draw $S \in \{S \subseteq N \mid |S| = l\}$ uniformly at random
    $\gamma \leftarrow v(S)$
    for $i \in S$ **do**
      $\hat{\phi}^+_{i,l-1} \leftarrow \frac{c_{i,l-1}\hat{\phi}^+_{i,l-1}+\gamma}{c^+_{i,l-1}+1}$
      $c^+_{i,l-1} \leftarrow c^+_{i,l-1} + 1$
    end for
    for $i \notin S$ **do**
      $\hat{\phi}^-_{i,l} \leftarrow \frac{c^-_{i,l}\hat{\phi}^-_{i,l}+\gamma}{c^-_{i,l}+1}$
      $c^-_{i,l} \leftarrow c^-_{i,l} + 1$
    end for
    $\hat{\phi}_i \leftarrow \frac{1}{n-\delta} \sum_{l=\delta}^{n-1} \hat{\phi}^+_{i,l} - \hat{\phi}^-_{i,l}, \forall i \in N$
  end while

3.3 Border Uncertainty Sampling

Kolpaczki et al. [KBH21] formally introduced the problem of identifying the Top-k Shapley players and proposed Border Uncertainty Sampling (BUS) (algorithm 3), an algorithm that focusses on players that are uncertain to belong to the top-k by calculationg their current estimated Shapley value's difference to the kth largest player's value. Although they did not provide mathematical proofs for its approximation quality, this method demonstrated promising empirical results.

In each iteration, the ordering $\hat{\pi} : N \to N$ is computed such that $\hat{\phi}_{\hat{\pi}(1)} \geq ... \geq \hat{\phi}_{\hat{\pi}(n)}$. The next player i to be updated is determined based on the lowest value of $\Delta_i \cdot t_i$, where Δ_i represents the difference between the player's current estimator and the kth largest value, and t_i is the number of times the player's marginal contribution has been updated. Intuitively the product represents the certainty of this player being classified correctly as part of the top-k or not. A player whose estimator is far away from the kth player's estimator and that has been updated many times is improbable to change partition while a player close to the kth player with rare updates is likely to cross the border between players in the top-k set and the remaining players.

This method fully capitalizes on the simplified problem statement by abstaining from wasting budget on players that are already confidently classified, instead improving the estimator of more uncertain players.
However, it still requires two value function calls per update, resulting in a budget efficiency of $\beta = \frac{1}{2}$. Unfortunately, easily adapting the concept of permutation sampling from ApproShapley, which allows for only one call per update, is not feasible as it relies on updating all player's Shapley values once per permutation.

Algorithm 3 Border Uncertainty Sampling

Require: $(N = \{1, .., n\}, v), k \in \mathbb{N}$
  $\hat{\phi}_i \leftarrow 0, t_i \leftarrow 0$, for all $i \in N$
  for $i \in N$ **do**
    Draw $S \subseteq N \setminus \{i\}$ with probability $\frac{1}{n\binom{n-1}{|S|}}$
    $\phi_i \leftarrow v(S \cup \{i\}) - v(S)$
  end for
  while $true$ **do**
    Compute $\hat{\pi} : N \to N$ with $\hat{\phi}_{\hat{\pi}(1)} \geq ... \geq \hat{\phi}_{\hat{\pi}(n)}$
    $\hat{\phi}^* \leftarrow \frac{\hat{\phi}_{\hat{\pi}(k)} + \hat{\phi}_{\hat{\pi}(k+1)}}{2}$
    $\Delta_i \leftarrow |\hat{\phi}_i - \hat{\phi}^*|, \forall i \in N$
    $p \leftarrow \arg\min_{i \in N} \Delta_i \cdot t_i$
    $t_p \leftarrow t_p + 1$
    Draw $S \subseteq N \setminus \{i\}$ with probability $\frac{1}{n\binom{n-1}{|S|}}$
    $\phi_{p,t_p} \leftarrow v(S \cup \{p\}) - v(S)$
    $\hat{\phi}_p \leftarrow \frac{(t_p - 1)\hat{\phi}_p + \phi_{p,t_p}}{t_p}$
  end while

3.4 Truncated Multi Armed Bandit Shapley

Ghorbani et al. [GZ20] propose the *Truncated Multi-Armed Bandit* (TMAB) Shapley algorithm, which builds upon the optimized version of Castro et al.'s ApproShapley [CGT09] also sampling permutations $O \in \pi(N)$. The TMAB algorithm enhances the approach by incorporating players' variances to compute confidence bounds for the estimators. Players whose confidence bounds do not cover the kth largest player's Shapley value are labeled as sufficiently approximated and are disregarded for the next iteration.

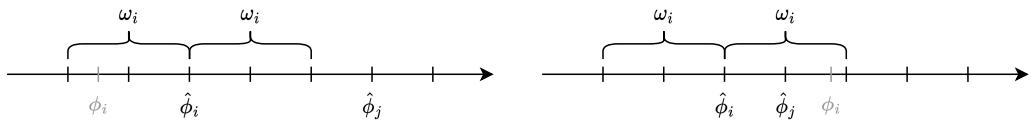
Example 3.4.1. Suppose we randomly sampled the permutation $O = (3, 4, 2, 1, 0)$ and players 2 and 4 have already been labeled as sufficiently approximated. When

iterating through the permutation as in ApproShapley, there is no need to calculate $v(2,1,0)$ since the only players whose marginal contribution would require this value are the players 2 and 4.

To determine the confidence bounds, the algorithm employs the empirical Bernstein method [MP09]. This ensures that with a probability of $1-\delta$ (where $\delta \in (0;1]$), the inequality

$$\phi_i - \hat{\phi}_i \leq \underbrace{\sqrt{\frac{2\sigma_i^2 \ln 2/\delta}{m}} + \frac{7 \ln 2/\delta}{3(m-1)}}_{:=\omega_i}$$

holds, where m denotes the number of samples used for the estimator $\hat{\phi}_i$ as in equation 2.3 and σ_i^2 represents the estimator's variance. This means that the player's estimator is at most ω_i off of its true value. Therefore, if the absolute difference between the estimors of this player and the kth largest player is larger than ω_i, the true Shapley value of the player is likely to be on the same side of the kth largest player as the estimator (see fig. 3.1) which indicates that the player is classified correctly and can be disregarded for now.



(a) $\hat{\phi}_j$ is outside the confidence bounds of player i. This suggests, that ϕ_i is also smaller than $\hat{\phi}_j$.

(b) $\hat{\phi}_j$ is inside the confidence bounds of player i. Therefore, ϕ_i might be greater than $\hat{\phi}_j$ even though $\hat{\phi}_i < \hat{\phi}_j$.

Fig. 3.1: Illustration of how the confidence bounds ω_i indicate whether the Shapley value of player i is certain to be smaller or greater than the Shapley value of player j.

In practice however, the algorithm tends to perform a large number of updates before players are excluded, as the confidence bounds can be quite high.

Example 3.4.2. Let's assume that all Shapley values fall between 0.01 and 0.02, and let $\delta = 0.2$. Even with a variance of zero, it would take at the very least 538 updates before a player is removed. This is because

$$\frac{7 \ln 2/0.2}{3(538-1)} \geq 0.01 = |0.01 - 0.02|$$

After 538 updates, the confidence bounds of this player still encompass all other players, including the kth largest one.

Initially, TMAB's budget efficiency is similar to ApproShapley, as all players are included. As the first players start to get exlcuded, the budget efficiency slightly decreases when the algorithm jumps over a set of players because when the next player is then evaluated the value function has to be called twice again.

As TMAB was developed for the Neuron Shapley application it employs a form of truncation aswell. Contrary to TruncStratSVARM, it doesn't use a fixed maximum coalition length but stops iterating through a permutation when the coalitions' values reach a certain threshhold v_T.
Algorithm 4 describes the TMAB Shapley algorithm by Ghorbani et al. [GZ20] with additional details compared to the original paper.

Remark 3.4.1. The authors did not evaluate their algorithm on a fixed budget scenario but rather allowed it to run until all players were excluded. To adapt the algorithm to our setting, we stop it when the budget is exhausted.

3.5 HybridApproBUS with Caching

In the first phase of BUS, a single marginal contribution is sampled for each player by means of a permutation in order to establish a foundation for uncertainty sampling in the next phase. However, we believe that obtaining a better approximation for all Shapley values initially would be more reasonable before focusing on updating only the uncertain players. In the initial iterations of uncertainty sampling, most players are equally uncertain, making it less significant to prioritize sampling the most uncertain player. Updating this player always requires two value function calls, which can be quite resource-intensive, especially considering that we do not benefit as much from BUS's strength in the beginning.
To address these issues, we propose a new algorithm called *HybridApproBUS*, where the initial warm-up phase is replaced by ApproShapley. Due to ApproShapley's better budget efficiency of $\beta = 1$ versus BUS's $\beta = \frac{1}{2}$ it is well-suited to create a first estimation for all Shapley values. We are repeating the more efficient sampling of permutations and specialize later with the uncertainty sampling as more and more players become irrelevant, rendering the permutation sampling less efficient. In order to determine when to transition from ApproShapley to BUS, we introduce a constant $s \in \mathbb{N}$ that defines the total amount of permutations that are iterated by

Algorithm 4 Truncated Multi Armed Bandit Shapley

Require: $(N = \{1, .., n\}, v), k \in \mathbb{N}, 0 < \delta \leq 1, v_T \in \mathbb{R}$
  $\hat{\phi}_i \leftarrow 0, \sigma_i^2 \leftarrow 0, S_i \leftarrow 0, \omega_i \leftarrow 0$, for all $i \in N$
  $t \leftarrow 0$
  $\mathcal{U} \leftarrow N$
  while $\mathcal{U} \neq \emptyset$ **do**
    $t \leftarrow t + 1$
    Draw $O \in \pi(N)$ uniformly with probability $\frac{1}{n!}$
    $v_0^t \leftarrow v(N)$
    for $i \in N$ **do**
      $p \leftarrow O(i)$
      if $p \in \mathcal{U}$ **then**
        if $v_{i-1}^t = null$ **then**
          $v_{i-1}^t \leftarrow v(\{O(i), ..., O(n)\})$
        end if
        if $v_{i-1}^t < v_T$ **then**
          $v_i^t \leftarrow v_{i-1}^t$
        else
          $v_i^t \leftarrow v(\{O(i+1), ..., O(n)\})$
        end if
        $S_p \leftarrow S_p + (v_{i-1}^t - v_i^t)^2$
        $\hat{\phi}_p \leftarrow \frac{(t-1)\hat{\phi}_p + v_{i-1}^t - v_i^t}{t}$
        $\sigma_p^2 \leftarrow \frac{S_p - t\hat{\phi}_p^2}{t-1}$
        $\omega_p \leftarrow \sqrt{\frac{2\sigma_p^2 \ln 2/\delta}{t}} + \frac{7 \ln 2/\delta}{3(t-1)}$
      else
        $v_i^t \leftarrow null$
      end if
    end for
    $\mathcal{U} \leftarrow \{i \mid \hat{\phi}_i - \omega_i < k\text{'th largest } \{\hat{\phi}_i\}_{i=1}^n < \hat{\phi}_i + \omega_i\}$
  end while

ApproShapley. In our evaluation we experiment with different values for s in order to find an optimal value.

Furthermore, we introduce *SmartHybridApproBUS* (algorithm 5), which incorporates a form of caching. Instead of sampling a coalition $S \subseteq N$, we sample permutations $O \in \pi(N)$ similar to ApproShapley. However, instead of iterating through the permutation, we determine the most uncertain player p as done in BUS. Like in ApproShapley we want to utilize permutation sampling to reuse coalition values. In order to do so, we use $E = (\epsilon_i)_{i=1}^n$ with $\epsilon_i \in \mathbb{R} \cup \{null\}$ to cache coalition values for the current permutation. Additionally, we maintain a binary indicator $w_i \in \mathbb{B}$ with $i \in N$ to track whether we have already calculated the marginal contribution of a player for the current permutation. If this is the case, the player's estimator has already been updated using this marginal contribution and a new permutation O has to be sampled. When calculating the marginal contribution of the selected player, we look up E to check if the required values are already cached and can be reused. If a coalition value is not cached, we evaluate it and store it in the cache.

Example 3.5.1. Consider the player set $N = \{1, 2, 3, 4\}$. Suppose we freshly sampled the permutation $(1, 2, 3, 4)$ and the cache $E = (null, null, null, null)$ is empty. Let's assume player 2 is currently the most uncertain player. The marginal contribution for player 2 can be calculated using $v(\{1, 2\}) - v(\{1\})$. After this calculation, the cache is updated, becoming $E = (v(1), v(1, 2), null, null)$. Now, if the next most uncertain player is player 1, for its marginal contribution $v(1) - 0$, we can reuse the value ϵ_1 from the cache. However, if the next most uncertain player is player 2 again, we must sample a new permutation since we already updated player 2 using the marginal contribution from this permutation.

3.6 HalfBUS

We propose a new algorithm, called HalfBUS (Algorithm 6), as an approximation method for computing the top-k Shapley values. Our algorithm is inspired by the works of Kolpaczki et al., specifically BUS [KBH21] and StratSVARM [KBH23]. While retaining the focus on players who are uncertain to belong to the top-k, HalfBUS improves budget efficiency by updating the Shapley values of multiple players with one sample, similar to StratSVARM.

Algorithm 5 SmartHybridApproBUS

Require: cooperative game $(N = \{1, .., n\}, v), k \in \mathbb{N}, s \in \mathbb{N}$
  $\hat{\phi}_i \leftarrow 0, t_i \leftarrow 0, \forall i \in N$
  for $r \leftarrow 1, ..., s$ **do**
    Take $O \in \pi(N)$ with probability $\frac{1}{n!}$
    $pre \leftarrow 0$
    for $i \in N$ **do**
      $p \leftarrow O(i)$
      $t_p \leftarrow t_p + 1$
      $\phi_{p,t_p} \leftarrow v(Pre^p(O) \cup \{p\}) - pre$
      $\hat{\phi}_p \leftarrow \frac{(t_p - 1)\hat{\phi}_p + \phi_{p,t_p}}{t_p}$
      $pre \leftarrow \phi_{p,t_p} + pre$
    end for
  end for
  Take $O \in \pi(N)$ with probability $\frac{1}{n!}$
  $\omega_i = false, \epsilon_i = null, \forall i \in \mathbb{N}$
  while $true$ **do**
    Compute $\hat{\pi} : N \to N$ with $\hat{\phi}_{\hat{\pi}(1)} \geq ... \geq \hat{\phi}_{\hat{\pi}(n)}$
    $\hat{\phi}^* \leftarrow \frac{\hat{\phi}_{\hat{\pi}(k)} + \hat{\phi}_{\hat{\pi}(k+1)}}{2}$
    $\Delta_i \leftarrow |\hat{\phi}_i - \hat{\phi}^*|, \forall i \in N$
    $p \leftarrow \arg\min_{i \in N} \Delta_i \cdot t_i$
    if $\omega_p = true$ **then**
      Take $O \in \pi(N)$ with probability $\frac{1}{n!}$
      $\omega_i = false, \epsilon_i = null, \forall i \in \mathbb{N}$
    end if
    $\omega_p \leftarrow true$
    get i with $O(i) = p$
    if $i = 0$ **then**
      $pre \leftarrow 0$
    else
      $pre \leftarrow \epsilon_{O(i-1)}$
    end if
    if $pre = null$ **then**
      $pre \leftarrow v(Pre^p(O))$
      $\epsilon_{O(i-1)} = pre$
    end if
    $curr \leftarrow \epsilon_p$
    if $curr = null$ **then**
      $curr \leftarrow v(Pre^p(O) \cup \{p\})$
      $\epsilon_p \leftarrow curr$
    end if
    $t_p \leftarrow t_p + 1$
    $\phi_{p,t_p} \leftarrow curr - pre$
    $\hat{\phi}_p \leftarrow \frac{(t_p - 1)\hat{\phi}_p + \phi_{p,t_p}}{t_p}$
  end while

Unlike BUS, which concentrates on the most uncertain player, HalfBUS identifies the set P of the w most uncertain players, ranging from 1 to n. Similar to StratSVARM, we draw a sample $S \subseteq N$ with probability $P(S) = \frac{1}{(n+1)\binom{n}{|S|}}$ and evaluate it using the value function. However, instead of updating all players using this value, we evaluate an additional coalition for each player $i \in P$. This coalition is selected in a way that its value forms a marginal contribution with $v(S)$ for player i. Specifically, if $i \in S$, we evaluate $v(S \setminus \{i\})$ and $v(S \cup \{i\})$ if $i \notin S$.

Our approach doesn't introduce a bias. This can be proven by reformulating eq. (2.1). Let $w_l = \frac{1}{n\binom{n-1}{l}}$ for $0 \leq l < n$. It is irrelevant if we sum over all coalitions that do not contain player i or if we sum over all coalitions that do contain player i and remove this player afterwards. Therefore:

$$\sum_{S \subseteq N, i \notin S} w_{|S|} \cdot [v(S \cup \{i\}) - v(S)] = \sum_{S \subseteq N, i \in S} w_{|S \setminus \{i\}|} \cdot [v(S) - v(S \setminus \{i\})].$$

Furthermore eq. (2.1) can be reformulated as:

$$\phi_i = \sum_{S \subseteq N} \begin{cases} \frac{1}{2} w_{|S|-1} \cdot [v(S) - v(S \setminus \{i\})], \text{ if } i \in S \\ \frac{1}{2} w_{|S|} \cdot [v(S \cup \{i\}) - v(S)], \text{ otherwise} \end{cases}. \tag{3.6}$$

Lemma 3.6.1. Given $i \in N$, the probability that a coalition $S \subseteq N$ drawn with distribution $P(S) = \frac{1}{(n+1)\binom{n}{|S|}}$ contains player i is $\frac{1}{2}$.

Proof:

$$\begin{aligned} P(i \in S) &= \sum_{l=0}^{n} P(i \in S, |S| = l) \\ &= \sum_{l=0}^{n} P(i \in S \mid |S| = l) \cdot P(|S| = l) \\ &= \sum_{l=0}^{n} \frac{\binom{1}{1}\binom{n-1}{l-1}}{\binom{n}{l}} \cdot \frac{1}{n+1} \\ &= \sum_{l=0}^{n} \frac{l}{n(n+1)} \\ &= \frac{1}{2} \end{aligned}$$

Theorem 3.6.1. By using eq. (3.6) to approximate the Shapley value of any player $i \in N$ we do not introduce a bias, i.e. $E(\hat{\phi}_i) = \phi_i$. Proof:
Given $i \in N$, let X denote a random variable with values $(x_S)_{S \subseteq N}$ where

$$x_S = \begin{cases} v(S) - v(S \setminus \{i\}), \text{ if } i \in S \\ v(S \cup \{i\}) - v(S), \text{ if } i \notin S \end{cases}$$

and probability distribution $P(X = x_S) = \frac{1}{(n+1)\binom{n}{|S|}}$. Then the expected value of X is:

$$\begin{aligned} E[X] &= \sum_{S \subseteq N} P(X = x_S) \cdot x_S \\ &= \sum_{S \subseteq N} \begin{cases} P(X = x_S, i \in S) \cdot [v(S) - v(S \setminus \{i\})], \text{ if } i \in S \\ P(X = x_S, i \notin S) \cdot [v(S \cup \{i\}) - v(S)], \text{ if } i \notin S. \end{cases} \end{aligned}$$

Using eq. (3.6) and:

$$\begin{aligned} P(X = x_S, i \in S) &= P(S \mid i \in S) \cdot P(i \in S) \\ &= \frac{1}{n\binom{n-1}{|S|-1}} \cdot \frac{1}{2} \\ &= \frac{1}{2} w_{|S|-1} \\ P(X = x_S, i \notin S) &= P(S \mid i \notin S) \cdot (1 - P(i \in S)) \\ &= \frac{1}{n\binom{n-1}{|S|}} \cdot \frac{1}{2} \\ &= \frac{1}{2} w_{|S|} \end{aligned}$$

we can show that $E[X] = \phi_i$.
By approximating this expected value using sampled coalitions $S \subseteq N$ as in eq. (2.3), we obtain an unbiased estimator for the Shapley value of player i.

The algorithm uses $w + 1$ value function calls for updating w players. Therefore the budget efficiency of HalfBUS is $\beta = \frac{w}{w+1}$. The choice of w depends on the application. When $w = 1$, HalfBUS essentially becomes BUS, as P contains only one player, and we require $1 + 1 = 2$ value function calls to update this player. On the other extreme, when $w = n$, we do not benefit from the uncertainty behavior of BUS, but we achieve the highest budget efficiency with n updates for $n + 1$ value function calls, similar to ApproShapley, which requires n calls for n updates.
We evaluate multiple versions of HalfBUS in order to find the ideal value for w.

Algorithm 6 HalfBUS

Require: cooperative game $(N = \{1, .., n\}, v), k \in \mathbb{N}, w \in N$
  $\hat{\phi}_i \leftarrow 0, t_i \leftarrow 0, \forall i \in N$
  $\gamma_n \leftarrow v(N)$
  while $true$ **do**
    Compute $\hat{\pi} : N \rightarrow N$ with $\hat{\phi}_{\hat{\pi}(1)} \geq ... \geq \hat{\phi}_{\hat{\pi}(n)}$
    $\hat{\phi}^* \leftarrow \frac{\hat{\phi}_{\hat{\pi}(k)} + \hat{\phi}_{\hat{\pi}(k+1)}}{2}$
    $\Delta_i \leftarrow |\hat{\phi}_i - \hat{\phi}^*|, \forall i \in N$
    Compute $\hat{\pi}' : N \rightarrow N$ with $\Delta_{\hat{\pi}'(1)} \cdot t_{\hat{\pi}'(1)} \leq ... \leq \Delta_{\hat{\pi}'(n)} \cdot t_{\hat{\pi}'(n)}$
    $P \leftarrow \{\hat{\pi}'(1), ..., \hat{\pi}'(w)\}$
    Take $l \in \{0, ..., n\}$ uniformly at random
    Take $S \subseteq N$ with $|S| = l$ uniformly at random
    if $l = n$ **then**
      $\gamma \leftarrow \gamma_n$
    else if $l = 0$ **then**
      $\gamma \leftarrow 0$
    else
      $\gamma \leftarrow v(S)$
    end if
    for $i \in P$ **do**
      $t_i \leftarrow t_i + 1$
      if $i \in S$ **then**
        $\phi_{i,t_i} \leftarrow \gamma - v(S \setminus \{i\})$
      else
        $\phi_{i,t_i} \leftarrow v(S \cup \{i\}) - \gamma$
      end if
      $\hat{\phi}_i \leftarrow \frac{(t_i - 1)\hat{\phi}_i + \phi_{i,t_i}}{t_i}$
    end for
  end while

4 Evaluation

4.1 Synthetic cooperative games

4.1.1 Experiment setup

We evaluate the different algorithms on synthetic cooperative games. These are cooperative games that are formulated in such a manner that the precise Shapley values can be computed within polynomial time. Synthetic games in which all players share identical Shapley values, such as the so called Gloves game, are not insightfull for comparing algorithms on the top-k problem. This limitation arises because all players fall within the top-k category, leading to a scenario where all algorithms exhibit 100% accuracy. To circumvent this issue, we employ the algorithms on synthetic games where players can be meaningfully categorized as either top-k players or not. In the following sections we present the chosen synthetic games for examination.

Sum of Unanimity Games

Definition 4.1.1 (Unanimity game)**.** Given a playerset $N = \{1, ..., n\}$ and a subgroup of players $R \subseteq N$, the cooperative game (N, v_R) using

$$v_R(S) = \begin{cases} 1 & \text{if } R \subseteq S, \\ 0 & \text{otherwise} \end{cases}$$

is called a *unanimity game*.

The unanimity game is a sort of voting game where a certain set of players has a right to veto, i.e. all of these players have to cooperate in order to achieve the reward. All players that do not belong to this subgroup are unimportant for the value

function making them dummy players. Therefore the total reward is distributed equally amongst the players in the veto group $i \in R$ each recieving a Shapley value of $\phi_i = \frac{1}{|R|}$.

Definition 4.1.2 (Sum of unanimity games)**.** Given a set of unanimity games $\{(N, v_{R_k})\}_{k=1}^{m}$, $m \in \mathbb{N}$ the linear combination of these games using weights $\{w_k\}_{k=1}^{m}$ is called a *sum of unanimity games* (SOUG) game. The value function is defined as:

$$v(S) = \sum_{k=1}^{m} w_k \cdot v_{R_k}(S)$$

The Shapley values of a SOUG game can be calculated by a linear combination of the Shapley values of the subgames, i.e.

$$\phi_i = \sum_{k=1}^{m} \begin{cases} \frac{w_k}{|R_k|} & \text{if } i \in R_k, \\ 0 & \text{otherwise} \end{cases}.$$

For our evaluation we generate random SOUG games. The parameters are drawn uniformly at random from the same ranges used by Kolpaczki et al. [KBH21]:

- $\{5, 6, ..., 50\}$ for the number of combined unanimity games m
- $\{0, 1, ..., n\}$ for the size of each R_k
- N for the members of each R_k
- $[0, \frac{1}{m}]$ for the weights w_k

Airport game

The *airport game* is the problem of distributing the cost of an airport's runway amongst the airplanes using this runway. Depending on the size of a plane i it requires a shorter or longer runway, represented by a cost c_i. The cost of a coalition of planes is the cost of the largest plane in this coalition as all smaller planes can use

the runway aswell. For a player set of planes $N = \{1, ..., n\}$ and costs $c_1, ..., c_n$ the value function of an airport games is defined as

$$v(S) = \max\{c_i \mid i \in S\}.$$

G. Owen [Owe13] provides a proof that the Shapley value of all planes can be calculated in polynomial time.
For our evaluation we use $N = \{1, ..., 100\}$ with costs

$$\begin{aligned} c_1, ..., c_{100} = &\underbrace{1, ..., 1}_{8 \text{ times}}, \underbrace{2, ..., 2}_{12 \text{ times}}, \underbrace{3, ..., 3}_{6 \text{ times}}, \underbrace{4, ..., 4}_{14 \text{ times}}, \underbrace{5, ..., 5}_{8 \text{ times}}, \\ &\underbrace{6, ..., 6}_{9 \text{ times}}, \underbrace{7, ..., 7}_{13 \text{ times}}, \underbrace{8, ..., 8}_{10 \text{ times}}, \underbrace{9, ..., 9}_{10 \text{ times}}, \underbrace{10, ..., 10}_{10 \text{ times}}. \end{aligned}$$

Castro et al. [CGT09] provide a list of precalculated Shapley values for this setting which we use in our evaluation.

Non-symmetric voting game

A *non-symmetric voting game* is a game where votes of different players i can have different weights w_i. In order for a coalition to win the reward of 1 it has to outweigh to opposing coalition of players. I.e. for a set of players $N = \{1, ..., n\}$ and weights $w_1, ..., w_n$ the value function is defined as

$$v(S) = \begin{cases} 1 & \text{if } \sum_{i \in S} w_i > \sum_{j \in N} w_j / 2, \\ 0 & \text{otherwise} \end{cases}.$$

For our evaluation we use a non-symmetric voting game by Castro et al. [CGT09] that mimics the voting process in the USA using $N = \{1, ..., 51\}$ and weights

$$\begin{aligned} w_1, ..., w_{51} = &45, 41, 27, 26, 26, 25, 21, 17, 17, 14, 13, 13, 12, 12, 12, 11, \\ &\underbrace{10, ..., 10}_{4 \text{ times}}, \underbrace{9, ..., 9}_{4 \text{ times}}, 8, 8, \underbrace{7, ..., 7}_{4 \text{ times}}, \underbrace{6, ..., 6}_{4 \text{ times}}, 5, \underbrace{4, ..., 4}_{9 \text{ times}}, \underbrace{3, ..., 3}_{7 \text{ times}}, \end{aligned}$$

They also provide a list of exact Shapley values which we reuse in our evaluation aswell.

4.1.2 Results

In this section we present the results of evaluating both the established and new algorithms on synthetic games. Like in fig. 4.1 we plot the average perfomance of an algorithm over a certain number of experiments (as explained in section 2.3) on the y-axis. The SE is visualized using a light shadow behind the line. The x-axis represents the budget that has been used up.

SmartHybridApproBUS implements the conjecture that the performance of BUS improves, if the Shapley values of the players are already reasonably approximated beforehand, which would make sorting for the most uncertain player more meaningfull.
To test this conjecture we run the algorithm using various different values for the switch parameter s indicating after how many iterations of ApproShapley we switch to BUS.

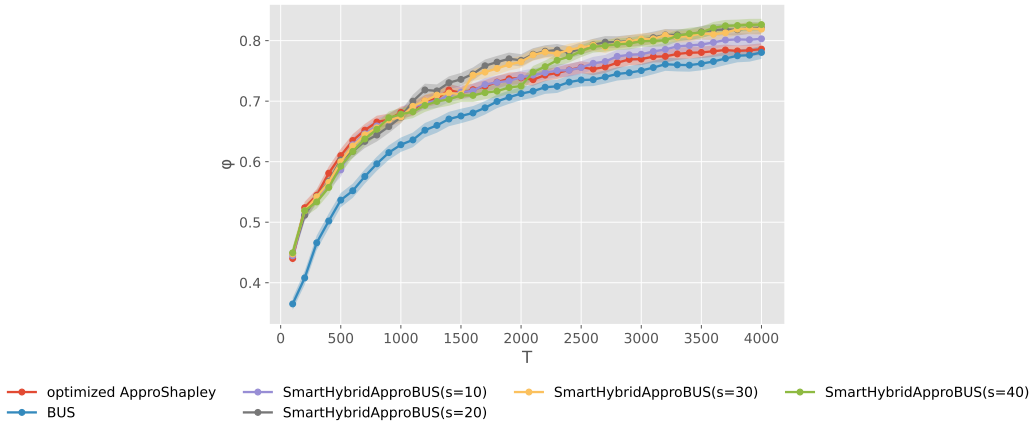


Fig. 4.1: Comparison of SmartHybridApproBUS with different values for s on SOUG games using $n = 50, k = 10$, averaged over 200 experiments

The results are depicted in fig. 4.1. We can see a significant improvement over BUS and ApproShapley for $s \geq 20$. For $s = 20, 30, 40$ we can observe a jump in performance at the point in time the algorithm switches to BUS (at $T = 1000, 1500, 2000$ respectively) which supports the theory. However, this effect of performance jump seems to be limited since all three versions end up on a similar line after $T = 3000$. This suggests that it helps BUS to have a proper estimation of the Shapley values first, to get a quick performance boost out of the uncertainty sampling, but from that point on the slope is similar to the original BUS algorithm.
For smaller values of s the effect is less significant. This suggests that the approximation of the values wasn't good enough to aquire the performance boost. We still

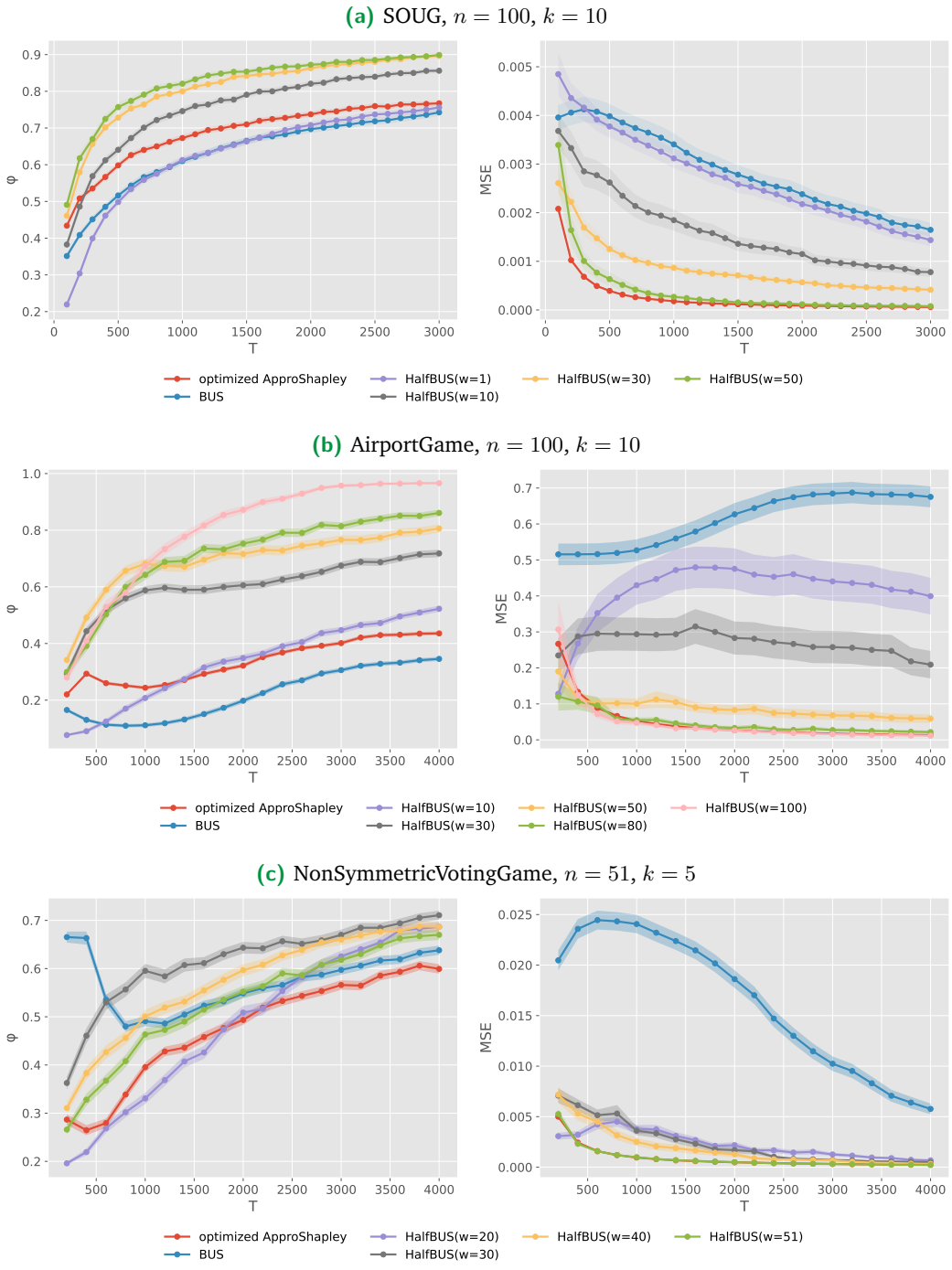


Fig. 4.2: Comparison of HalfBUS with different values for w on diffent games, averaged over 300 experiments

see a slight improvement over BUS and ApproShapley which is probably due to the caching. The caching itself doesn't result in a strong increase in performance which is not surprising since the cached values are rarely used. Since BUS mostly focusses

on a small set of uncertain players, a sample cannot be reused very often.

HalfBUS is supposed to improve the budget efficiency of BUS by updating the marginal contribution of a set of uncertain players instead of a single one. This way the value of a single sample can be reused multiple times. As shown in fig. 4.2, we tested HalfBUS on multiple synthetic games using varying values for w, which specifies the length of the selected set of players to be updated in each iteration. As expected, visible in fig. 4.2a, using $w = 1$ HalfBUS achieves a very similar result to BUS as it becomes basically the same algorithm. All other variants perform far better than both BUS and ApproShapley. Interestingly though, in most experiments it seems that choosing $w = n$ achieves the best results. This is surprising, because using $w = n$ basically removes the uncertainty sampling of the algorithm as all players are updated in each iteration. It also has a very similar budget efficiency to ApproShapley, infact even a slightly worse one of $\beta = \frac{w}{w+1}$ versus ApproShapley's $\beta = 1$ which is why we would expect it to perform similar to ApproShapley. As the plots for the MSE show, this is exactly what is happening for the approximation problem. ApproShapley and HalfBUS have a very similar curve for $w = n$ with the one of HalfBUS being slightly worse. The decrease in budget efficiency should be negligible, when using a value of w only slightly smaller than n. However, in fig. 4.2b for example, *HalfBUS(w=100)* performs significantly better than *HalfBUS(w=80)*. Both have similar budget efficiency of $\frac{100}{101} \approx 0.99 \approx \frac{80}{81}$. This suggests, that another factor apart from budget efficiency or uncertainty sampling plays a part here.

We suppose, the main reason for HalfBUS's performance increase over ApproShapley and BUS is the fact that in each iteration all players of the selected set recieve an update using coalitions with similar sizes and consisting of mostly the same players, which makes comparing their values much more reasonable in contrast to updating each player with a random coalition. For the approximation problem this doesn't matter because each player's estimated value is solely compared to its own exact value and not the other players.
Asssuming that this is actually the reason for HalfBUS's performance increase in the top-k problem, this would also explain why choosing smaller values than n for w and taking advantage of uncertainty sampling doesn't yield even better results. This is because only the players in the selected set are updated using similar coalitions while the rest is not, which negatively influences the ability to compare players of these seperate sets. When using $w = n$ all players always recieve an update using a similar coalition in each iteration making all values comparable.

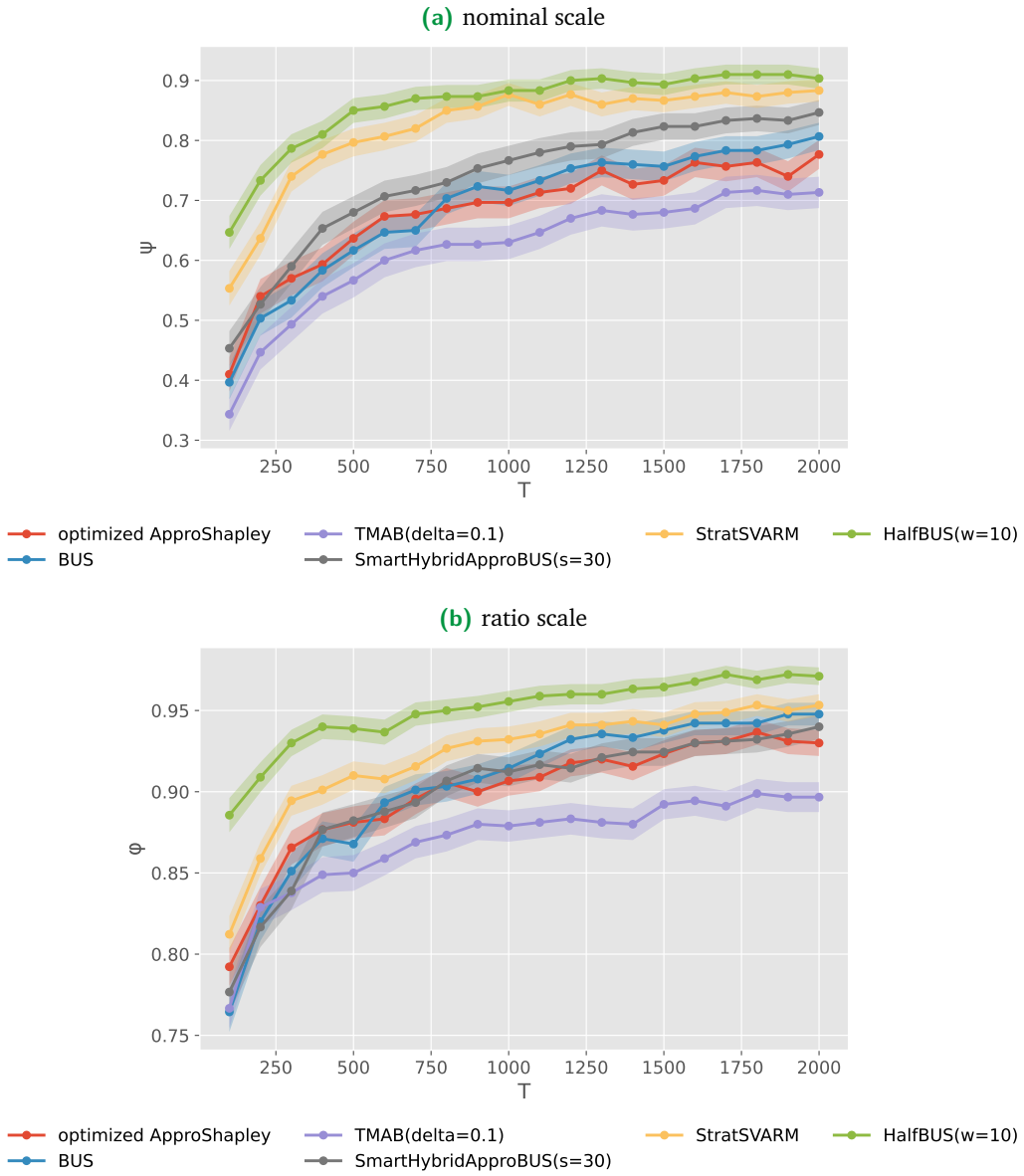


Fig. 4.3: Comparison of all algorithms on SOUG games using $n = 10, k = 3$, averaged over 300 experiments

Next we compare our algorithms using the optimal parameters to the remaining algorithms of chapter 3. Figures 4.3 to 4.5 show the experiments we conducted. Figure 4.3a mimics the SOUG experiment of Kolpaczki et al. [KBH21] as they use a nominal scale aswell. The results of BUS are slightly better in our experiment, which we suppose is due to the fact that their problem statement assumes the set of top-k players to be unique.

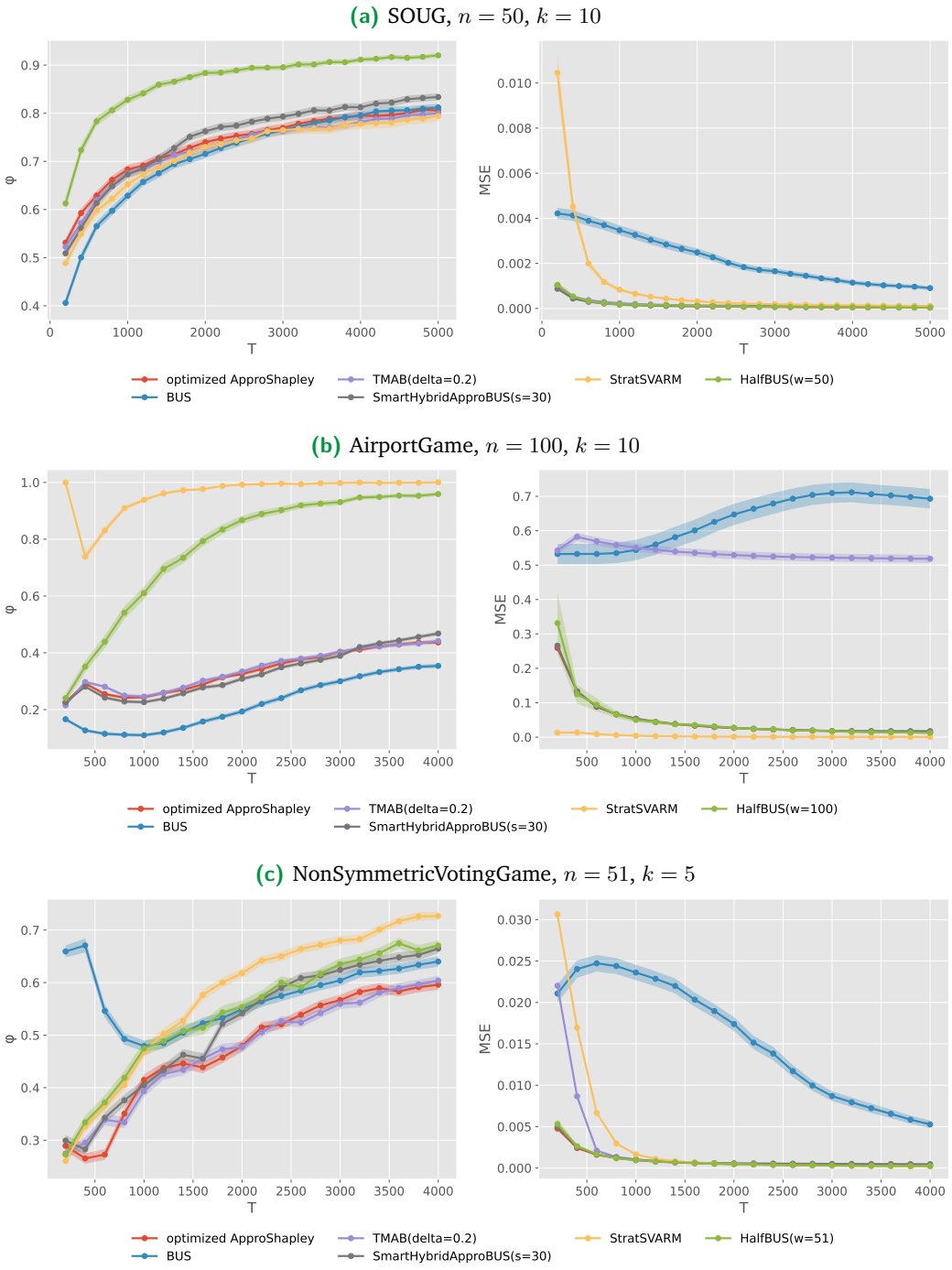


Fig. 4.4: Comparison of all algorithms on different games, averaged over 300 experiments

In fig. 4.4 we evaluate all algorithms in the different synthetic games using medium sized player sets. SmartHybridApproBUS seems to perform slightly better than ApproShapley and BUS but it does not achieve groundbreaking improvements. Ghorbani et al.'s TMAB algorithm [GZ20] performs almost identically to ApproShapley.

As explained in section 3.4, this is due to the fact that the confidence bounds used in the algorithm do not come into play for such a low budget. Since the value of synthetic games does not approach zero for small coalitions we disabled truncation for TMAB. With these limitations, TMAB differs only slightly from ApproShapley. HalfBUS on the other hand yields far better results than most algorithms, especially in the SOUG and the AirportGame. The only other algorithm that achieves similar or even better results is Kolpaczki et al.'s Stratified SVARM [KBH23] which is not surprising considering it has by far the best budget efficiency out of all algorithms. At least for fig. 4.4a the sampling strategy of HalfBUS, updating all players using similar coalitions seems to outweigh StratSVARM's budget efficiency.
However, StratSVARM's budget efficiency increases proportional to the size of the player set which is why we conducted the SOUG experiment using larger values of n visible in fig. 4.5.

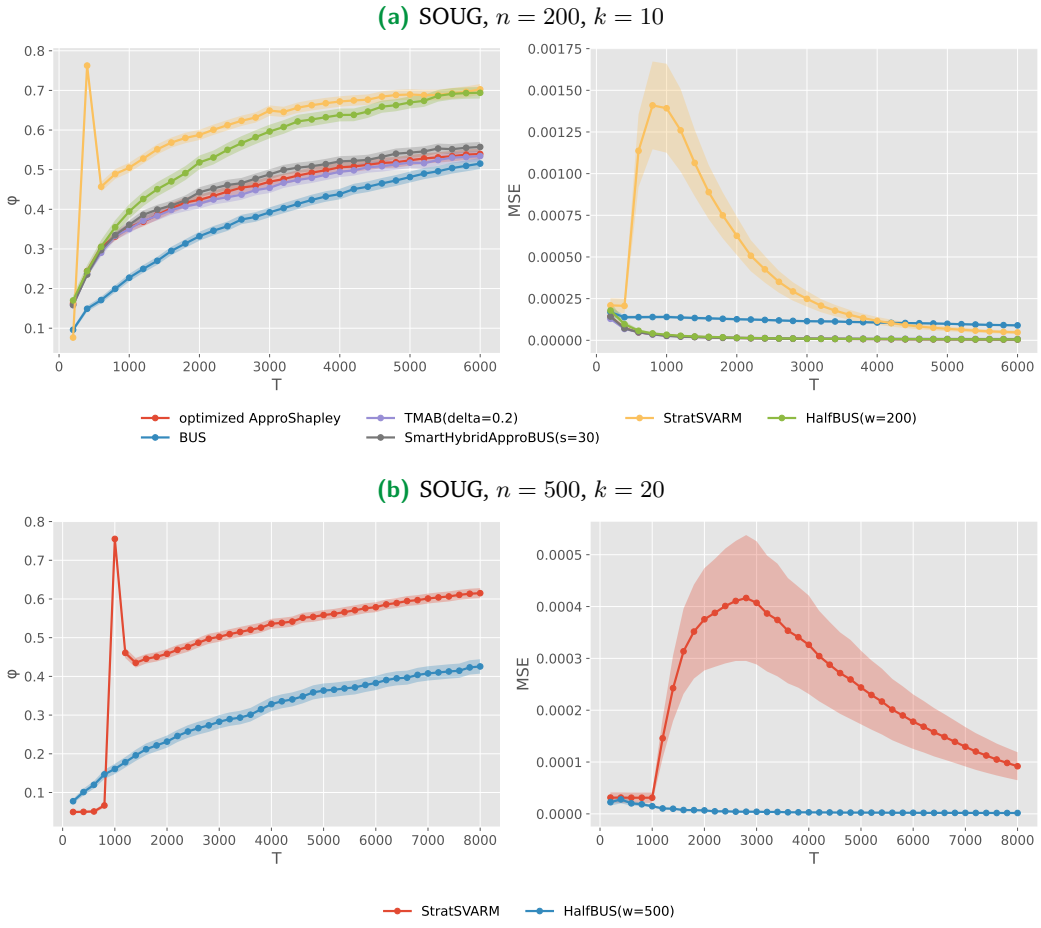


Fig. 4.5: Evaluation on larger player sets, averaged over 300 experiments

As expected, compared to the other algorithms the performance of StratSVARM increases with the size of the player set. For $n = 200$ it performs slightly better than HalfBUS where HalfBUS can still catch up in the end. However, for $n = 500$ StratSVARM clearly outperforms HalfBUS.
The spike of StratSVARM's curve at the beginning comes from the exact calculation part where the exact values for the stratas of length $0, 1, n-1$ and n are calculated which apperently already results in an accurate ordering of the players in SOUG games. The drop in performance afterwards is due to the fact, that StratSVARM doesn't update whole marginal contributions, which makes the approximation inaccurate at the beginning as the coalitions used to update $\hat{\phi}^+$ might not be easily comparable to the coalitions used to update $\hat{\phi}^-$. This effect is also tracked by the MSE in fig. 4.5. However, the comparison between φ and the MSE also shows that the performance of an algorithm on the top-k problem is not neccessarily strongly correlated to its approximation accuracy.

Remark 4.1.1 (Computational expense of StratSVARM). Since StratSVARM updates all players with each sample, it requires way more computational power compared to the other algorithms. Even though we tried to optimize the code for updating the players as much as possible it requires roughly five times the amount of time to finish compared to the rest. The experiment in fig. 4.5b took over five hours for StratSVARM while HalfBUS finished in just over an hour. The increased memory requirements of StratSVARM are also significant.

4.2 Measuring Pixel Importance

In XAI, it is desirable to understand how a model arrived at a certain conclusion. In the case of image detection we are interested in which pixels influenced the model the most in making a specific decision.
To identify these influential pixels, we can create a feature selection game by treating each pixel as a player and using the model's performance as the value function.

4.2.1 Experiment setup

We trained a simple linear neural network on the Fashion-MNIST dataset [XRV17] to classify images of clothing into 10 categories: 'T-Shirt', 'Trouser', 'Pullover', 'Dress', 'Coat', 'Sandal', 'Shirt', 'Sneaker', 'Bag', and 'Ankle Boot'. The model consists of an input layer with 784 neurons (one for each pixel in the 28x28 image), one hidden layer with 512 neurons, and an output layer with 10 neurons (one for each class). We achieved an overall test accuracy of 71.9%.
When running the model on a sampled image, such as in Fig. 4.6, it can correctly classify the item as a coat.
We create the cooperative game where each of the 784 pixels represents a player.

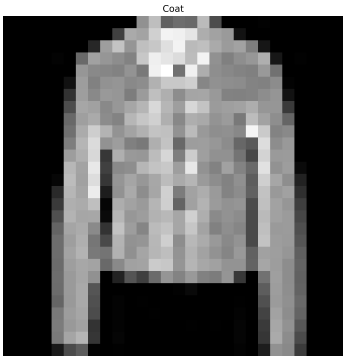


Fig. 4.6: Sample from the Fashion MNIST test dataset: Coat

The value function takes a coalition of players and runs the model with the remaining pixels being zeroed out. However, merely setting these values to zero (resulting in black pixels) would not be sufficient since black pixels can still carry information just like white pixels. To address this, we replace the zeroed-out pixels with their average value in the dataset, as illustrated in fig. 4.7. This kills the information

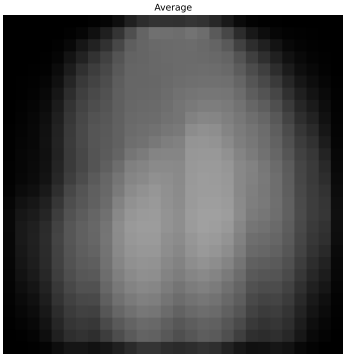


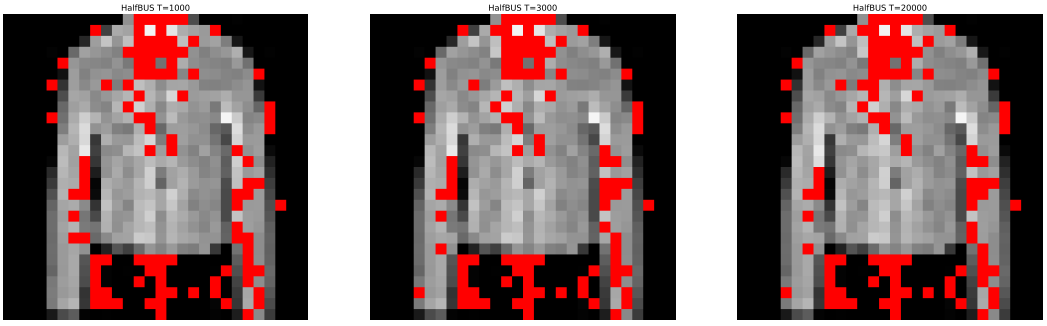
Fig. 4.7: Average pixel values of Fashion MNIST test dataset

of this pixel. In order to quantify the model's performance on the sampled image

with partially zeroed out pixels we calculate the cross entropy loss using the model's output and the actual value. Since the loss decreases as the model's performance improves, the value function returns the inverse of the loss. To ensure that $v(\emptyset) = 0$ when no pixels are included, we subtract the value of running the model with all pixels zeroed out. In practice this wouldn't be neccessary since we do not care about the exact Shapley values, only the top-k players.

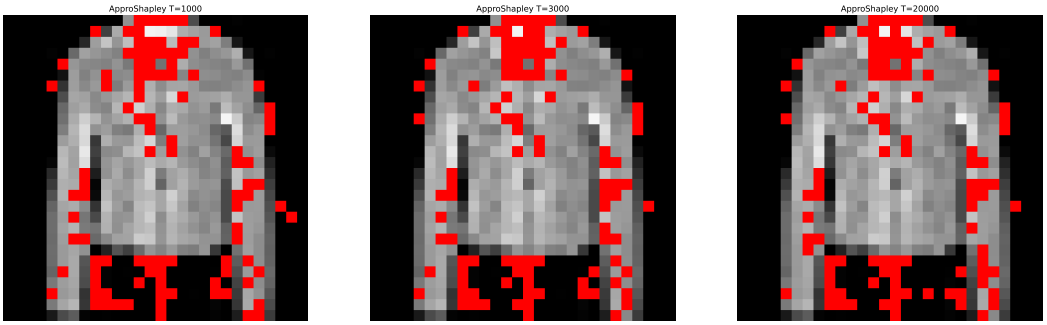
4.2.2 Results

We evaluate the feature selection game on HalfBUS using $w = 100$, along with the optimized version of ApproShapley and Stratified SVARM, as shown in figs. 4.8 to 4.10. We are unable to plot the algorithms' performances as we do not know the actual top-k players. Correctly identifying them would require the evaluation of all 2^{784} coalitions which we are unable to carry out. However, by running the algorithms for longer and comparing these results to outputs with smaller budegts we get an indication on how fast the model is able to identify the top-k.



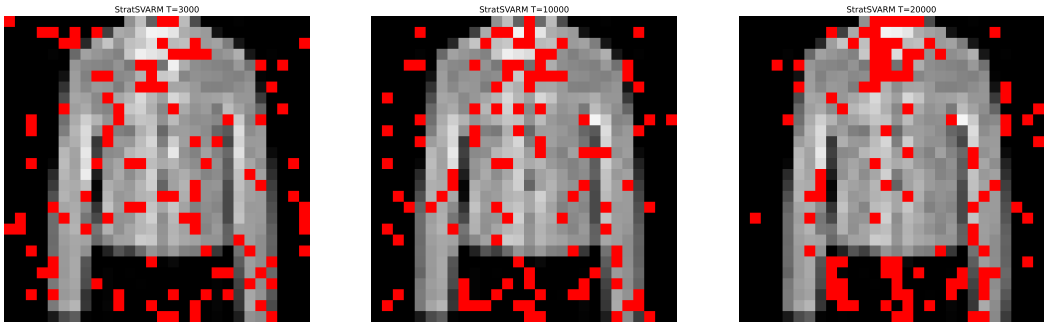
(a) $T = 1000$ **(b)** $T = 3000$ **(c)** $T = 20000$

Fig. 4.8: Resulting top-100 pixels (red) of HalfBUS with Budget T using $w = 100$



(a) $T = 1000$ **(b)** $T = 3000$ **(c)** $T = 20000$

Fig. 4.9: Resulting top-100 pixels (red) of optimized ApproShapley with Budget T



(a) $T = 3000$ **(b)** $T = 10000$ **(c)** $T = 20000$

Fig. 4.10: Resulting top-100 pixels (red) of StratSVARM with Budget T

The red pixels indicate the top 100 pixels identified by the algorithms for the sampled image of a coat.
Upon inspecting the results, it appears that the model focuses primarily on the area around the neck, the contours of the coat, and the black area at the bottom. The latter may be crucial in distinguishing it from, for example, a dress, which is usually longer.
Notably, HalfBUS delivered the best results, as after only 1000 value function calls, it seems to provide a good estimation of the top-100 pixels as its selection only changes slightly when running it up to a budget of 20000.
ApproShapley achieved a very similar result to HalfBUS after 20000 calls, which strongly suggests that these results accurately describe the actual top-100 pixels. However, it seems to perform slightly worse than HalfBUS, as its selection varies slightly up to a budget of 3000.
On the other hand, Stratified SVARM doesn't seem to perform well, as its selection appears to be quite random. Only after around 20000 calls do the selected pixels start to group together similarly to the other results.

4.3 Neuron Shapley

4.3.1 Experiment setup

We try to replicate some of the experiments conducted by Ghorbani et al. [GZ20]. The authors focused on CNNs applied on image detection.

In the first experiment we try to identify a set of critical neurons in the Inception-v3 [Sze+16] model using different algorithms. The used model is trained on the ImageNet dataset ILSVRC2012 [Rus+15]. Like Ghorbani et al. [GZ20] we split the ImageNet test dataset in a validation set and a test set where the validation set is used to calculate Shapley values. The model achieves an accuracy of 76.8% on our test set. Similar to Ghorbani et al. [GZ20] we create a cooperative game where the 17216 convolutional filters of the model (excluding the last layer, also called logit layer) represent the player set. The accuracy of the model, evaluated on a batch of 64 images, is chosen as an approximation for the value function. In theory, to get a well defined result for the value function the accuracy of the model on the whole validation dataset would have to be calculated. This however, would dramatically increase the runtime which is not feasable for our hardware constraints. Ghorbani et al. approximate the value aswell using a batch size of 128. Coalitions of players are formed by "zeroing" the remaining players. Players are zeroed by fixing their output to their average output as explained in section 2.4.2. We run the algorithms on this cooperative game and evaluate their performance by zeroing the identified top-k players and evaluating the model's accuracy on the test dataset. If the algorithm successfully identified highly important neurons, the accuracy of the model should drop. Additionally, we evaluate how strongly the model is impacted when the players with the lowest Shapley values are removed.

Ghorbani et al. [GZ20] test whether it is possible to fix a NN's bias by removing the responsible neurons. They trained the SqueezeNet [Ian+16] architecture on the celeba [Liu+18] dataset to detect the gender from face images and achieve a test accuracy of 98%. Similar to the Inception model we use the 2976 convolutional filters as players and the model's accuracy on a batch of 256 images as the value function. We tried to recreate this setting but are only able to achieve a test accuracy of 97.1%, possibly due to minimal deviating model constructions which is a result of missing documentation of the authors. The model is tested on a different dataset to test whether it has a certain bias towards certain races. As we where not able to get access to the PPB dataset [BG18] as used by Ghorbani et al. we use the FairFace dataset [KJ21] as it has an equal representation of different ethnicities aswell. We try to recreate Ghorbani et al.'s experiment [GZ20], where the Shapley values are calculated using the dataset with fair representations of all ethnicities and test if the model's performance increases or biases are removed when the harmfull players are removed.
Additionally we calculate the Shapley values on a single ethnicity in order to target a certain bias explicitly by removing the worst players again.

Ghorbani et al. [GZ20] run their experiments using a cluster of 100 computing machines each with 12 CPU cores taking a total of 21 hours per experiment. In our setting this is equivalent to a budget of $T \approx 45000000$. Due to hardware limitations we are only able to allow for a budget of $T = 50000$ per experiment.

4.3.2 Results

We remove the top-10 and top-100 Shapley players of the Inception model calculated using the algorithms HalfBUS, TMAB, and TruncStratSvarm. For HalfBUS we implement a simple form of truncation aswell, similar to TruncStratSvarm. For both algorithms we ignore coalitions of sizes smaller than 16000. Removing up to 100 neurons from the model only barely impacts its accuracy if chosen randomly. The results are shown in fig. 4.11.

Not surprisingly, HalfBUS and TMAB are not able to identify highly important neurons using a budget of only $T = 50000$. Due to their budget efficiency and the total number of players of 17216 both are only able to update each player a few times. TruncStratSvarm however, is able to impact the model's performance already using a budget of $T = 20000$ and completely diminishes its accuracy after removing the top-10 players after 50000 calls. This is a major improvement over the results of Ghorbani et al. [GZ20]. Using TMAB they where only able to drop the model's accuracy on their test set from 74% to 38% and used a budget of roughly $T \approx 45000000$. TruncStratSvarm is able to drop the model's accuracy on our test set from 76.8% to 15.7% using $T = 50000$ which is just a fraction of the author's budget. This can be explained using TruncStratSvarm's budget efficiency being proportional to the number of players. After 50000 calls, each player is updated 25000 times while Ghorbani et al. reportedly ran the algorithm for 3000 iterations which roughly equals 3000 updates per player considering TMAB has a similar budget efficiency to ApproShapley. This way we are able to produce better results than Ghorbani et al. [GZ20], even with a way lower budget. Figure 4.12 shows the results of removing the worst-k players of the model. Again TruncStratSvarm perfoms the best, retaining a lot of the model's accuracy, even after removing 1000 players.

Our SqueezeNet model, trained on the celeba dataset, is able to achieve an accuracy of 74.2%. Unlike Ghorbani et al. [GZ20] we are not able to increase the model's performance by removing the worst neurons with any of the algorithms. Neither did the accuracy increase for a minority group.

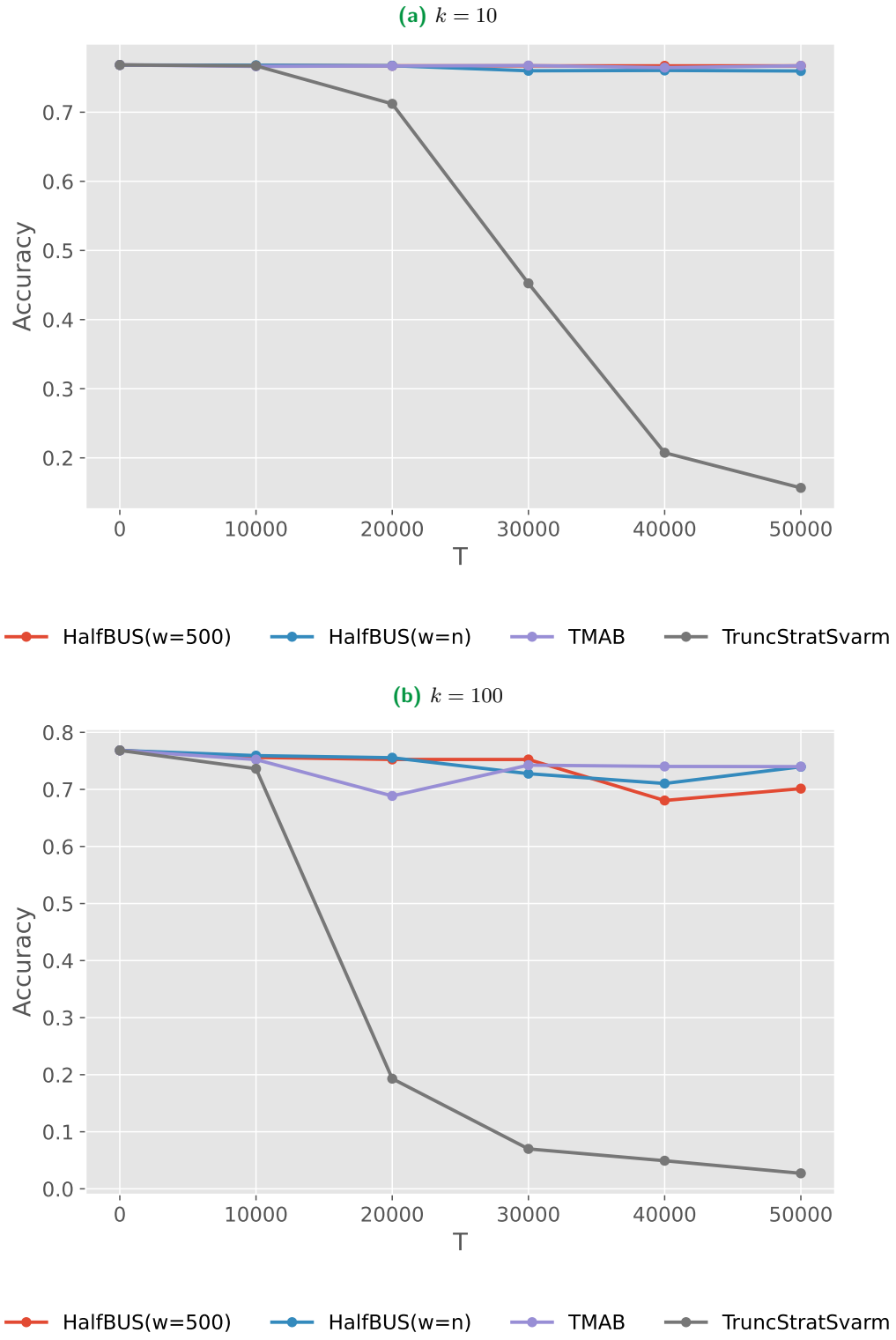


Fig. 4.11: Performance comparison of Inception model after removing the top-k players identified by different algorithms.

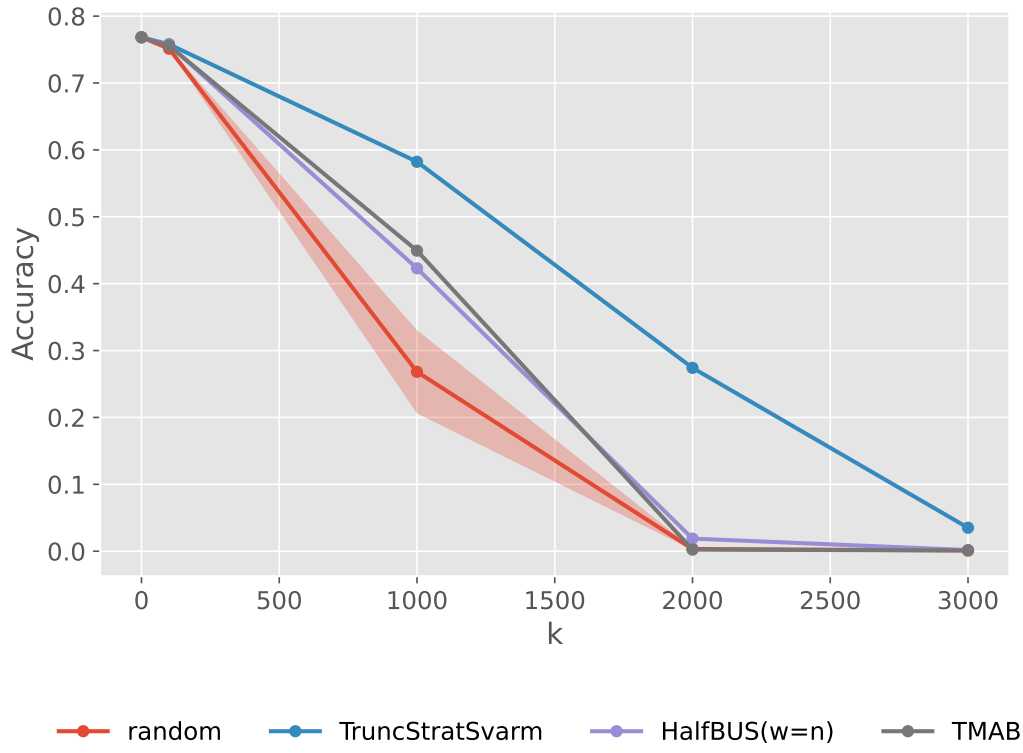


Fig. 4.12: Performance comparison of Inception model after removing the worst-k players identified by different algorithms using a budget of $T = 50000$.

However, we conducted a second experiment. The models performance was the worst for faces of people from southeast asia with an accuracy of 70.0%. We tried to specifically target this bias by calculating the Shapley values only using faces of this ethnicity. We were able to increase to models accuracy on that minority group. Removing the worst 3 neurons, results in an accuracy of 71.3% for TruncStratSvarm, 71.4% for HalfBUS and 71.1% using TMAB on this minority while the accuracy on the whole dataset dropped to 71.7% for TruncStratSvarm and 73.7% for HalfBUS. Using TMAB the accuracy on the whole dataset even slightly increased to 74.8%. All these results however, are not as significant as those by Ghorbani et al. [GZ20]. Since the authors used a different dataset it is hard to compare the results. Possibly, the data of FairFace is too different to the celeba dataset to even apply the model meaningfully.

5 Conclusion and future work

In this thesis we gave an overview about of Shapley values and the more specific Top-k Shapley player problem and its applications in XAI. We tested state of the art approximation algorithms on the top-k problem and investigated new ideas by introducing the algorithms SmartHybridApproBUS and HalfBUS. We evaluated all algorithms thoroughly in order to find core mechanisms that have a strong impact on an algorithm's performance on the top-k problem.
Although there's not one algorithm that performs best across all test cases, StratSVARM by Kolpaczki et al. [KBH23] and HalfBUS tend to achieve the best results. For the application of applying Shapley values to the neurons in a neural network in order to detect highly important neurons StratSVARM is the clear winner. The reason is its budget efficiency that increases proportional to the amount of players. For smaller player sets however, HalfBUS achieved the best results. Even though StratSVARM still has a better budget efficiency, HalfBUS shows that the way the Shapley values are approximated plays an important role aswell. While for the approximation problem all players can be approximated independently as they are solely compared to their real value, for the top-k problem the players need to be compared by their size. Thus approximating all players using similar coalitions as done in HalfBUS has a strong positive effect on comparability even with a lower budget efficiency.

By applying TruncStratSVARM on a neural network in order to identify the most important neurons we were able to achieve even better results than Ghorbani et al.'s TMAB with a budget several magnitudes lower. The reason again is Stratified SVARM's budget efficiency. With our set budget of 50000 in each experiment TruncStratSVARM was able to update every player's average marginal contribution 25000 times while Ghorbani et al. [GZ20] even with a budget of roughly 45000000 were only able to update each player about 3000 times as TMAB's budget efficiency is similar to the optimized version of ApproShapley.
In addition we were able to conduct our experiments on a single GPU in comparison to Ghorbani et al. [GZ20] who used a cluster of 100 computing machines with 12 CPU cores each.

In the future it might be reasonable to investigate on the behaviour of HalfBUS

further as it demonstrates that for the top-k problem the factor of comparability between the players' estimators plays an important role. This aspect has not drawn much attention yet as it is irrelevant with regards to the approximation problem alone. Therefore, we strongly suggest taking this factor into account for future top-k algorithm research.

Bibliography

[Agg+18] Charu C Aggarwal et al. “Neural networks and deep learning”. In: *Springer* 10.978 (2018), p. 3 (cit. on pp. 10, 11).

[Bro+20] Tom Brown, Benjamin Mann, Nick Ryder, et al. “Language models are few-shot learners”. In: *Advances in neural information processing systems* 33 (2020), pp. 1877–1901 (cit. on pp. 1, 2, 10).

[BG18] Joy Buolamwini and Timnit Gebru. “Gender shades: Intersectional accuracy disparities in commercial gender classification”. In: *Conference on fairness, accountability and transparency*. PMLR. 2018, pp. 77–91 (cit. on p. 44).

[CGT09] Javier Castro, Daniel Gómez, and Juan Tejada. “Polynomial calculation of the Shapley value based on sampling”. In: *Computers & Operations Research* 36.5 (2009), pp. 1726–1730 (cit. on pp. 3, 16, 21, 33).

[GZ20] Amirata Ghorbani and James Y Zou. “Neuron shapley: Discovering the responsible neurons”. In: *Advances in Neural Information Processing Systems* 33 (2020), pp. 5922–5932 (cit. on pp. 3, 8, 13, 14, 21, 23, 38, 43–45, 47, 49).

[HB18] Ayanna Howard and Jason Borenstein. “The ugly truth about ourselves and our robot creations: the problem of bias and social inequity”. In: *Science and engineering ethics* 24 (2018), pp. 1521–1536 (cit. on p. 2).

[Ian+16] Forrest N Iandola, Song Han, Matthew W Moskewicz, et al. “SqueezeNet: AlexNet-level accuracy with 50x fewer parameters and< 0.5 MB model size”. In: *arXiv preprint arXiv:1602.07360* (2016) (cit. on pp. 13, 44).

[KJ21] Kimmo Karkkainen and Jungseock Joo. “FairFace: Face Attribute Dataset for Balanced Race, Gender, and Age for Bias Measurement and Mitigation”. In: *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision*. 2021, pp. 1548–1558 (cit. on p. 44).

[KBH23] Patrick Kolpaczki, Viktor Bengs, and Eyke Hüllermeier. “Approximating the shapley value without marginal contributions”. In: *arXiv preprint arXiv:2302.00736* (2023) (cit. on pp. 3, 6, 7, 18, 19, 25, 39, 49).

[KBH21] Patrick Kolpaczki, Viktor Bengs, and Eyke Hüllermeier. “Identifying Top-k Players in Cooperative Games via Shapley Bandits.” In: *LWDA*. 2021, pp. 133–144 (cit. on pp. 3, 8, 9, 20, 25, 32, 37).

[KSH12] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. “Imagenet classification with deep convolutional neural networks”. In: *Advances in neural information processing systems* 25 (2012) (cit. on p. 1).

[LBH15] Yann LeCun, Yoshua Bengio, and Geoffrey Hinton. “Deep learning”. In: *nature* 521.7553 (2015), pp. 436–444 (cit. on p. 1).

[Liu+18] Ziwei Liu, Ping Luo, Xiaogang Wang, and Xiaoou Tang. “Large-scale celebfaces attributes (celeba) dataset”. In: *Retrieved August* 15.2018 (2018), p. 11 (cit. on p. 44).

[LL17] Scott M Lundberg and Su-In Lee. “A unified approach to interpreting model predictions”. In: *Advances in neural information processing systems* 30 (2017) (cit. on p. 12).

[MP09] Andreas Maurer and Massimiliano Pontil. “Empirical bernstein bounds and sample variance penalization”. In: *arXiv preprint arXiv:0907.3740* (2009) (cit. on p. 22).

[Mio+18] Riccardo Miotto, Fei Wang, Shuang Wang, Xiaoqian Jiang, and Joel T Dudley. “Deep learning for healthcare: review, opportunities and challenges”. In: *Briefings in bioinformatics* 19.6 (2018), pp. 1236–1246 (cit. on p. 1).

[Mol20] Christoph Molnar. *Interpretable machine learning*. Lulu. com, 2020 (cit. on pp. 3, 12).

[Owe13] Guillermo Owen. *Game theory*. Emerald Group Publishing, 2013 (cit. on p. 33).

[Ram+22] Aditya Ramesh, Prafulla Dhariwal, Alex Nichol, Casey Chu, and Mark Chen. “Hierarchical text-conditional image generation with clip latents”. In: *arXiv preprint arXiv:2204.06125* (2022) (cit. on pp. 10, 11).

[Roz+22] Benedek Rozemberczki, Lauren Watson, Péter Bayer, et al. “The shapley value in machine learning”. In: *arXiv preprint arXiv:2202.05594* (2022) (cit. on p. 2).

[Rus+15] Olga Russakovsky, Jia Deng, Hao Su, et al. “Imagenet large scale visual recognition challenge”. In: *International journal of computer vision* 115 (2015), pp. 211–252 (cit. on p. 44).

[Sel+17] Sreelekshmy Selvin, R Vinayakumar, EA Gopalakrishnan, Vijay Krishna Menon, and KP Soman. “Stock price prediction using LSTM, RNN and CNN-sliding window model”. In: *2017 international conference on advances in computing, communications and informatics (icacci)*. IEEE. 2017, pp. 1643–1647 (cit. on p. 1).

[Sha+53] Lloyd S Shapley et al. “A value for n-person games”. In: *Princeton University Press Princeton* (1953), pp. 307–317 (cit. on pp. 2, 5).

[Sze+16] Christian Szegedy, Vincent Vanhoucke, Sergey Ioffe, Jon Shlens, and Zbigniew Wojna. “Rethinking the inception architecture for computer vision”. In: *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016, pp. 2818–2826 (cit. on pp. 13, 44).

[Vas+17] Ashish Vaswani, Noam Shazeer, Niki Parmar, et al. “Attention is all you need”. In: *Advances in neural information processing systems* 30 (2017) (cit. on p. 1).

[XRV17] Han Xiao, Kashif Rasul, and Roland Vollgraf. “Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms”. In: *arXiv preprint arXiv:1708.07747* (2017) (cit. on p. 41).

Webpages

[@AI22] Stability AI. *Stable Diffusion Launch Announcement*. 2022. URL: `https://stability.ai/blog/stable-diffusion-announcement` (visited on Aug. 11, 2023) (cit. on p. 10).

[@Wei03] Eric W Weisstein. *Sample variance*. 2003. URL: `https://mathworld.wolfram.com/` (visited on July 20, 2023) (cit. on p. 10).

List of Figures

Colophon

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Munich, February 4, 2022

Tim Nielen