Piecewise Approximations of Black Box Models for Model Interpretation

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Abstract

Recent literature interprets the predictions of “black-box” machine learning models (Neural Networks, Random Forests, etc.) by approximating these models in terms of simpler models such as piecewise linear or piecewise constant models. Existing literature does not provide guarantees on whether these approximations reflect the nature of the predictive model well, which can result in poor interpretations thus establishing mistrust in the model. We provide a *tractable* dynamic programming algorithm that partitions the feature space into subsets and assigns a local model (constant/linear model) to provide piecewise constant/piecewise linear interpretations of an arbitrary predictive model. When approximation loss (between the interpretation and the predictive model) is measured in terms of mean squared error, our approximation is optimal; for more general loss functions, our interpretation is approximately optimal, i.e., it probably approximately correctly (PAC) learns the predictive model. Experiments with real and synthetic data show that it provides significant improvements (in terms of mean squared error) over competing approaches. We also show real use cases to establish the utility of the proposed approach over competing approaches.

1 Introduction

Machine Learning algorithms have proved extremely successful for a wide variety of supervised learning problems. However, in some domains, adoption of these algorithms has been hindered because the “black-box” nature of these algorithms makes their predictions difficult or impossible for potential users to interpret. This issue is especially important in the medical domain and security applications Caruana et al. (2015). European Union’s Law on Data Regulation taking effect in 2018 Goodman and Flaxman (2016) makes it mandatory for “black-box” models to explain how they arrive at the predictions before implementing them in practice.

The problem of interpretation has received substantial attention in the literature recently (discussed below) Ribeiro et al. (2016) Shrikumar et al. (2017) Bastani et al. (2017) Chen et al. (2018). These papers have approached the problem of interpreting the black box model by approximating it with *piecewise models* (e.g., piecewise constant or piecewise linear) (See the justification in Lundberg and Lee (2017)). [1] Approximating a black box model in terms of a piecewise model is useful to determine the following:

- **Instancewise feature importance:** Identify the importance assigned by the black box to the different features when making a prediction for a certain instance Chen et al. (2018). Black box models based on neural networks, random forests etc, have been proposed to replace the existing risk scores (based on linear models, decision trees, etc.) in clinical practice Weng et al. (2017). Providing the clinician access to these importance scores helps the clinician understand the model, establish trust, and also debug the model in some cases.
- **Phenotypes:** Instancewise feature importance only provides insights into the model at a local level Bastani et al. (2017) Yang et al. (2018), while understanding the model at a global level is very important to establish trust. It is impractical to provide the feature importance associated with all the data instances. Hence, it is important to identify subsets of datapoints with different feature importances Yang et al. (2018) such that within each

[1] We define piecewise models later.

subset the feature importances are similar. Different subsets (with similar feature importances) belong to different pieces in a piecewise model (as we will see later). In medical terminology, these subsets are called "phenotypes" Kim et al. (2017).

In Figure 1, we show an example of a black-box model that predicts the risk of heart failure based on age and weight. We identify three phenotypes, where each phenotype corresponds to a risk interval, low risk, medium risk and high risk. In each interval, we use a fixed linear model to approximate the black-box model. The coefficients associated with age and weight vary significantly for the three phenotypes as shown. Further details can be explored in `https://mlinterpreter.shinyapps.io/app_try/`

Existing works on model interpretation that use piecewise models to approximate the global model Bastani et al. (2017) Ribeiro et al. (2016) often do not search the space of the piecewise models effectively and can often result in poor approximations. As a result, the resulting interpretation may poorly reflect the true nature of the black-box (discussed later in Section 7.2). In general, searching for the best [2] piecewise approximation is non-trivial (justification provided later) and we address this problem in this work. Due to space limitation, we do not provide a detailed account of related works here and instead give them in the Supplementary Material.

Contribution In this paper we propose piecewise interpreter (PI), to interpret the black-box models. Our method is to use the black-box predictive model and a given data set to construct a partition of the feature space into subsets and to assign a simple local model to each subset. We propose a dynamic programming based approach to find the partition of the dataset and the set of local models. We prove that the output of PI is approximately optimal in several different cases, i.e. it PAC learns the predictive model. We use several real and synthetic datasets to show that the proposed approach results in significantly better interpretable model approximations compared to competing approaches. We use real medical datasets to show how existing approaches can mislead the user in believing that the black box model does not use certain important risk factors that are well known clinically while infact it actually does use those factors.

2 Problem Formulation

We are given a space $\mathcal{X}$ of *features* and a space $\mathcal{Y} = [0,1]^d$ of *labels*. We are given a predictive model $f : \mathcal{X} \rightarrow \mathcal{Y}$ (say a random forest based model or a deep neural network model). The data is distributed according to some *true distribution* $\mathcal{D}$ (typically unknown) on $\mathcal{X}$. Our objective is to interpret f in terms of *interpretive models*, which are defined below. We seek to find a interpretive model that approximates f.

Interpretive models: The intepretive models we consider here represent the most commonly used models in literature on model interpretation Ribeiro et al. (2016)Lundberg and Lee (2017). The interpretive models we consider are defined by partitioning $\mathcal{X}$ into a finite number of disjoint sets and assigning a simple model (linear or constant model) to each set of the partition (In the Supplementary Material we describe how many models in literature belong to this category).

To make this precise, recall that a (finite) partition of a subset $A \subset \mathcal{X}$ is a family $\mathcal{Z} = \{Z_1, Z_2, \ldots, Z_K\}$ of subsets of $\mathcal{X}$ such that $\bigcup_{i=1}^{K} Z_i = A$ and $Z_i \cap Z_j = \emptyset$ if $i \neq j$. Given a partition $\mathcal{Z}$ of A and a feature $a \in A$ we write $\mathcal{Z}(a)$ for the index of the unique element of the partition $\mathcal{Z}$ to which a belongs. Write $\mathcal{P}(A)$ for the set of all (finite) partitions of A and $\mathcal{P}_K(A)$ for the set of partitions having at most K elements. We define $\mathcal{M} = \{M_1, ..., M_K\}$ a set of local models, where model M_j corresponds to the local model for points in Z_j. Each local model M_j belongs to a set $\mathcal{H}$ of models, where $\mathcal{H}$ can be from the family of constant models ($M_j(x) = c$, where $c \in \mathbb{R}^d$) [4] or linear models ($M_j(x) = Bx + c$, where $B \in \mathbb{R}^{d \times |\mathcal{X}|}$ and $c \in \mathbb{R}^d$) [5].

Given a partition $\mathcal{Z}$ of $\mathcal{X}$ and the corresponding set of local models $\mathcal{M}$, we define a *interpretive model* $g_{M,\mathcal{Z}} : \mathcal{X} \rightarrow Y$ by $g_{\mathcal{M},\mathcal{Z}}(x) = M_{\mathcal{Z}(x)}(x)$.

Loss functions: We measure the goodness of fit of a proposed interpretation g for f in terms of a given *loss function* (for e.g., mean squared error). We assume $\ell : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a continuous, strictly increasing, strictly convex function such that $\ell(0) = 0$. We define the risk achieved by model $g_{M,\mathcal{Z}}$ as follows

$$R(f, g_{M,\mathcal{Z}}; \mathcal{D}) = E_{\mathcal{D}}[l(\|f(X) - g_{M,\mathcal{Z}}(X)\|_s)] \qquad (1)$$

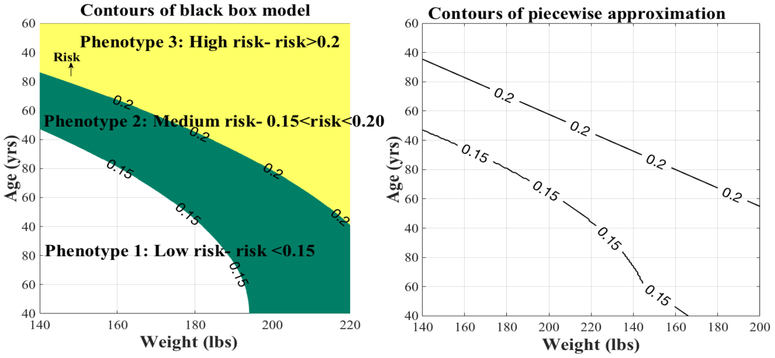
where X is a feature from the distribution $\mathcal{D}$, the expectation is taken over the distribution $\mathcal{D}$, and $\|.\|_s$ is the s-norm.

Risk Minimization: We impose an upper bound K on the number of sets in a partition (provided as input by the clinician). Our objective is to find a partition $\mathcal{Z}$ and a map $M : \mathcal{Z} \mapsto \mathcal{Y}$ (where each local model is drawn from $\mathcal{H}$) to minimize the true risk subject to the constraint that the size of the partition, i.e., $|\mathcal{Z}| \leq K$.

$$(\mathcal{M}^*, \mathcal{Z}^*) = \underset{\mathcal{M} \in \mathcal{H}^K, \mathcal{Z} \in \mathcal{P}_K(\mathcal{X})}{\operatorname{argmin}} R(f, g_{M,\mathcal{Z}}; \mathcal{D}) \qquad (2)$$

$g_{M^*,\mathcal{Z}^*}$ is the best piecewise model that minimizes the above risk.

[2] The notion of optimality is defined later.



Phenotype	Rank	Coefficient (Weight, Age)
Low risk	Weight > Age	(0.67, 0.46)
Medium risk	Age > Weight	(1, 2)
High risk	Age > Weight	(3.5, 4.6)

Figure 1: Comparison of the black box model versus the piecewise approximation. White, Green and Yellow colored regions represent three different phenotypes. Coefficients of the features and the associated ranking is also shown.

Empirical Risk Minimization: In practice, we do not know the true distribution $\mathcal{D}$ so we cannot minimize the true risk; instead, we see only a finite dataset (training set) $D = \{x_i\}_{i=1}^N$ drawn from the true distribution. For given $\mathcal{M}, \mathcal{Z}$ the empirical risk is

$$\hat{R}(\mathcal{M}, \mathcal{Z}; D) = \frac{1}{n} \sum_{x_i \in D} \left[l(\|f(x_i) - g_{M,\mathcal{Z}}(x_i)\|_s) \right] \quad (3)$$

The spirit of Probably Approximately Correct (PAC) learning Shalev-Shwartz and Ben-David (2014) suggests that we should minimize the empirical risk:

$$(\mathcal{M}^\dagger, \mathcal{Z}^\dagger) = \underset{\mathcal{M} \in \mathcal{H}^K, \mathcal{Z} \in \mathcal{P}_K(\mathcal{X})}{\operatorname{argmin}} \hat{R}(\mathcal{M}, \mathcal{Z}; D) \quad (4)$$

Later we will show that solving the above empirical risk minimization problem is PAC solution to the actual risk minimization problem in (2). We cannot solve the above problem using brute force search because it requires searching among $\mathcal{O}(|D|^K)$ partitions, which becomes intractable very quickly with increase in $|D|$ and K. In the next section, we propose an Algorithm to solve the above problem.

3 Piecewise Interpreter Algorithm

In this section, we develop the Piecewise Interpreter Algorithm to solve the problem discussed above. Without loss of generality we assume that all the data points x_i in D are sorted in the increasing order of the norm of $f(x_i)$, i.e. $\|f(x_i)\|$.

We give a summary of the working of the Algoirthm next. We give a detailed analysis of the Algorithm in Section 4 and 5. There are two parts to the Algorithm (Algorithm 1 and 2). In the first part, the Algorithm partitions the data D into subsets and finds an optimal local model corresponding to each subset. The division of the dataset into these subsets relies on dynamic programming. Suppose that the Algorithm wants to divide the first p points into q subsets. Also, suppose that the Algorithm has already constructed a partition to divide the first m points into k subsets for all $m \leq p-1$ and for all $k \leq q-1$. The risk achieved by partition of m points where the size of the partition is k is defined as $V(m,k)$. For each $x_i \in D, x_j \in D$, where $i \leq j$, define a subset of the data as follows.

$$D(i,j) = \{x : x \in D \ \& \ \|f(x_i)\| \leq \|f(x)\| \leq \|f(x_j)\|\}$$

We define the optimal local model on $D(i,j)$ as follows

$$G(i,j) = \min_{h \in \mathcal{H}} \frac{1}{|D(i,j)|} \sum_{x_r \in D(i,j)} \left[l(\|f(x_r) - h(x_r)\|_s) \right]$$

$$M(i,j) = \underset{h \in \mathcal{H}}{\operatorname{argmin}} \frac{1}{|D(i,j)|} \sum_{x_r \in D(i,j)} \left[l(\|f(x_r) - h(x_r)\|_s) \right]$$

The Algorithm constructs a partition to divide p points into q subsets as follows

$$V(p,q) = \min_{n' \in \{1,..,p-1\}} \left[V(n', q-1) + G(n'+1, p) \right]$$

$$\Phi(p,q) = \underset{n' \in \{1,..,p-1\}}{\operatorname{argmin}} \left[V(n', q-1) + G(n'+1, p) \right]$$

where $\Phi(p, q)$ is the index of the first data point in the q^{th} subset. The subset q consists of all the points indexed $\{\Phi(p, q), ..p\}$. The model for the q^{th} subset is $M(\Phi(p, q) + 1, p)$. Similarly, the next subset, i.e., the q^{th} subset can be computed recursively as $\{\Phi(\Phi(p, q), q - 1), .., \Phi(p, q) - 1\}$ and so on. In the first part of the Algorithm, we construct a partition of D and the corresponding set of local models. In the second part of the Algorithm, we extend this partition from the dataset D to the set $\mathcal{X}$. We write the function that is output by the Algorithm 2 as $g_{M^{\#},\mathcal{Z}^{\#}}$.

4 Main Results

Our goal in this section is to show that the output of the Algorithm PAC learns f and the Algorithm computes $g_{M^{\#},\mathcal{Z}^{\#}}$ in polynomial time. We begin by computing the computational complexity of the Algorithm. We assume that the loss function is the mean squared error and we assume that the local models are drawn from the constant model class. In the Supplementary Material, we show that for other norms and other local model classes as well the complexity is cubic in $|D|$.

Complexity of Algorithms 1 and 2

Theorem 1. The computational complexity of Algorithm 1 and 2 together is $\mathcal{O}(|D|^3 Kd)$.

The Proof of Theorem 1 is given in the Supplementary Material. While $\mathcal{O}(|D|^3 Kd)$ is much better than the brute force search among $\approx |D|^K$ ordered partitions, it can still be large. Hence, we propose some speed-ups (in the Supplementary Material) and used them in the Numerical Results Section.

PAC learnability of Algorithms 1 and 2: In this section, we discuss whether the outcome of Algorithm 1 and 2, i.e. $g_{M^{\#},\mathcal{Z}^{\#}}$ PAC learns f.

Assumption 1: We assume that family of local models $\mathcal{H}$ corresponds to the set of constant models, i.e. the interpretive models are piecewise constant.

Assumption 2: We also assume that if $\|f(x_i)\| < \|f(x_j)\| \implies f(x_i) < f(x_j)$, i.e., $f(x_j)$ Pareto dominates $f(x_i)$. If f is scalar, i.e., $f(x)) \in [0, 1], \forall x \in \mathcal{X}$, then the above assumption always holds.

For the next theorem, let Assumption 1 and 2 be true. In the next section, we discuss the optimality for piecewise linear models.

Theorem 2 $\forall \epsilon > 0, \delta \in (0, 1), \exists\ n^*(\epsilon, \delta)$ such that if D is drawn i.i.d. from $\mathcal{D}$ and $|D| \geq n^*(\epsilon, \delta)$, then with probability at least $1 - \delta$,

$$|R(f, g_{\mathcal{M}^{\#},\mathcal{Z}^{\#}}; \mathcal{D}) - R(f, g_{\mathcal{M}^*,\mathcal{Z}^*}; \mathcal{D})| \leq \epsilon$$

The proof of Theorem 2 is given in the Supplementary Material.

4.1 Piecewise linear models

In Theorem 2, we assumed that the local model is constant. In this section, we discuss Theorem 2 in the context of piecewise linear models. We divide the discussion into two parts.

First, suppose that we use a linear model as the local model in Algorithm 1 and 2, then it is hard to show PAC learnability as in Theorem 2. However, if we restrict the set of partitions we search to a special class of partitions, i.e., ordered partitions, that we define in Section 5.1, then we can extend Theorem 2 to this setting as well (See the Piecewise Linear Models Section in Supplementary Material).

Second, in many cases, we only require that the interpretation to be able to predict the importances that a model associates with different features, i.e., the gradient of the black-box w.r.t the features. Suppose that the outcome of the black-box is a scalar, i.e., $d = 1$ and suppose that the black-box model f is differentiable w.r.t x almost everywhere. In this case, instead of finding a piecewise linear interpretive model that minimizes the distance w.r.t f, we can find an interpretive model that minimizes the distance w.r.t the gradient of f, i.e., ∇f. We know that the gradient of a piecewise linear function is defined almost everywhere and corresponds to a piecewise constant function. Hence, we can use a piecewise constant model that explains ∇f. Therefore, we can apply Theorem 2 and conclude that the interpretive model PAC learns the gradient of f.

We summarize the results for the piecewise constant function and piecewise linear models in Table 1.

5 Principles Underlying the Main Results and the Algorithm

In this section, we first describe the principles behind the construction of the Algorithm and then we develop the propositions that lead up to the main result discussed in Section 4. In Section 5.1, we identify a new class of partitions that we call *ordered partitions* and restrict our search in that space. The empirical risk function defined earlier follows Bellman principle when we restrict the search spac. In Section 5.2, we show that the dynamic programming approach presented in Algorithm 1 and 2 searches for the optimal ordered partition. In Section 5.3, we show that the risk achieved by the optimal ordered partition and the corresponding models found by the proposed algorithm is very close to the risk achieved by the optimal partition $\mathcal{M}^{\dagger}, \mathcal{Z}^{\dagger}$ defined in (4). We then use results on PAC learning Shalev-Shwartz and Ben-David (2014) and certain properties of the family of piecewise functions to establish the main result Theorem 2.

Algorithm 1 Computing value and index functions

```
Input: Dataset $D$, Number of subsets $K$
Initialize: Define $V^{'}(1,k) = 0, \forall k \in \{1,...,K\}$.
For each $x_i \in D, x_j \in D$ such that $i \leq j$, define $D(i,j) = \{x : x \in D \text{ and } \|f(x_i)\| \leq \|f(x)\| \leq \|f(x_j)\|\}$
$G(i,j) = \min_{h\in\mathcal{H}} \frac{1}{|D(i,j)|} \sum_{x_r \in D(i,j)} \left[l(\|f(x_r) - h(x_r)\|_s)\right]$
$M(i,j) = \arg\min_{h\in\mathcal{H}} \frac{1}{|D(i,j)|} \sum_{x_r \in D(i,j)} \left[l(\|f(x_r) - h(x_r)\|_s)\right]$
for  $n \in \{2,...,|D|\}$ do
    for $k \in \{1,...,K\}$ do
        $V^{'}(n,k) = \min_{n^{'} \in \{1,..,n-1\}} \left[V^{'}(n^{'}, k-1) + G(n^{'}+1, n)\right] \quad (5)$
        $\Phi(n,k) = \operatorname{argmin}_{n^{'} \in \{1,..,n-1\}} \left[V^{'}(n^{'}, k-1) + G(n^{'}+1, n)\right] \quad (6)$
Output: Value function $V^{'}$, Index function $\Phi$
```

Algorithm 2 Computing partitions using the index function

```
Input: Index function $\Phi$, Black box predictive model $f$
Initialization: $h_u = |D|$
for  $k \in \{1,...,K\}$ do
        $h_l = \Phi(h_u, K-k+1)$
        $Z_{K-k+1} = \{x : \|f(x_{h_l})\| < \|f(x)\| \leq \|f(x_{h_u})\|\}$
        $M_{K-k+1} = M(h_l+1, h_u)$
        $h_u = h_l$

Output: $\mathcal{Z}^{\#} = \{Z_1,...,Z_K\}$,
$\mathcal{M}^{\#} = \{M_1,...,M_K\}$
```

5.1 Ordered Partitions

We say that the partition $\mathcal{Z}$ of $A \subset \mathcal{X}$ is *ordered* if for every $Z, Z' \in \mathcal{Z}$ with $Z \neq Z'$, either

(i) for all $z \in Z, z' \in Z'$ we have $\|f(z)\| < \|f(z')\|$, or

(ii) for all $z \in Z, z' \in Z'$ we have $\|f(z)\| > \|f(z')\|$

Write $\mathcal{P}^*(A)$ for the set of all ordered partitions of A and $\mathcal{P}^*_K(A)$ for the set of all ordered partitions of A having at most K (non-empty) elements. We now show that the risk defined over the partitions follows the Bellman principle. Let $\mathcal{Z}$ be a partition of $A \subset \mathcal{X}$ and let $\mathcal{Z}', \mathcal{Z}'' \subset \mathcal{Z}$ be a partition of $\mathcal{Z}$; i.e. $\mathcal{Z}' \cup \mathcal{Z}'' = \mathcal{Z}$ and $\mathcal{Z}' \cap \mathcal{Z}'' = \emptyset$.

Bellman Principle Let $\mathcal{Z}$ be an ordered partition of $\mathcal{X}$, $\mathcal{M}$ be the set of optimal local models, and assume that $\hat{R}(\mathcal{M}, \mathcal{Z}; D)$ minimizes the risk among all ordered partitions of $\mathcal{X}$ with at most $|\mathcal{Z}|$ elements. If $\mathcal{Z}', \mathcal{Z}'' \subset \mathcal{Z}$ is a partition of $\mathcal{Z}$, $\mathcal{M}', \mathcal{M}'' \subset \mathcal{M}$ is a partition of $\mathcal{M}$, then $\hat{R}(\mathcal{M}^{'}, \mathcal{Z}'; D)$ minimizes the risk among all ordered partitions of A' with at most $|\mathcal{Z}'|$ elements. If this were not true then we could find another ordered partition $\mathcal{Z}^*$ of A' with lower risk. But then $\mathcal{Z}^* \cup \mathcal{Z}''$ would be an ordered partition of $\mathcal{X}$ with lower risk than $\mathcal{Z}$, which would be a contradiction.

5.2 Optimal Ordered Partitions

In this section, we will show that the Algorithm conducts a search in the space of ordered partitions and finds the solution that minimizes the objective in (4).

Proposition 1. The output of the Algorithm 1 and 2 achieves a risk value equal to $\min_{M,\mathcal{Z}\in\mathcal{P}^*_K(\mathcal{X})} \hat{R}(M, \mathcal{Z}; D)$.

The proof of Proposition 1 is given in the Supplementary Material. We give a brief proof sketch next. In the first part, the Algorithm constructs a value function and an index function; the second part uses the value function and the index function to produce an ordered partition. We use induction and Bellman principle. Suppose we consider the first p points and we want to partition them into q subsets. Suppose that the optimal partitions for the first m points into k subsets is known $\forall m \leq p-1$ and $\forall k \leq q-1$. From Bellman principle, we know that the risk achieved by the optimal partition of p points into q subsets is equal to $\min_{n^{'}\in\{1,..,m\}} \left[V(n^{'}, q-1) + G(n^{'}+1, p)\right]$. From the construction of the Algorithm it follows that the partition of p points into q subsets computed by the Algorithm is optimal because the risk achieved by it is equal to $\min_{n^{'}\in\{1,..,m\}} \left[V(n^{'}, q-1) + G(n^{'}+1, p)\right]$.

5.3 Optimal Ordered Partitions are Optimal Among all Partitions

We have shown that the ordered partitions constructed in Algorithms 1 and 2 are optimal among ordered partitions; we justify our focus on ordered partitions

Table 1: Summary of results on PAC learnability for different settings

Interpretive Model	**Set of Partitions**	**Shape-penalty**	**Risk function**	**Output**
Piecewise constant	All & size $\leq K$	No	$E\big[l(\lVert f - g_{\mathcal{M},\mathcal{Z}}\rVert)\big]$	PAC learns f
Piecewise linear	Ordered &size $\leq K$	No	$E\big[l(\lVert f - g_{\mathcal{M},\mathcal{Z}}\rVert)\big]$	PAC learns f
Piecewise linear	All & size $\leq K$	No	$E\big[l(\lVert \nabla f - \nabla g_{\mathcal{M},\mathcal{Z}}\rVert)\big]$	PAC learns ∇f
Piecewise constant/linear	Ordered & size $\leq K$	Yes	$E\big[l(\lVert f - g_{\mathcal{M},\mathcal{Z}}\rVert) + penalty\big]$	PAC learns f

by demonstrating their optimality *among all partitions*. We invoke Assumptions 1 and 2 from Section 4 for the next two propositions.

Proposition 2. If the loss function is mean squared error then $\min_{\mathcal{M},\mathcal{Z}\in\mathcal{P}_K(\mathcal{X})} \hat{R}(\mathcal{M},\mathcal{Z};D) = \min_{\mathcal{M},\mathcal{Z}\in\mathcal{P}^*_K(\mathcal{X})} R(\mathcal{M},\mathcal{Z};D)$

The proof of Proposition 2 is in the Supplementary Material. In the next Proposition, we consider more general loss functions unlike the Proposition 2.

In the general case in which the loss function is only strictly convex, we show that the risk achieved by optimal ordered partitions is *probably approximately* the minimal risk over arbitrary partitions.

Proposition 3. For every $\epsilon, \delta > 0$ and every K there is some $m^*(\epsilon,\delta,K)$ such that if the training set D is drawn i.i.d. from the distribution $\mathcal{D}$ and $|D| \geq m^*(\epsilon,\delta,K)$, then with probability at least $1-\delta$ we have $\big|\min_{\mathcal{Z}\in\mathcal{P}_K(\mathcal{X})} R(\mathcal{M},\mathcal{Z};D) - \min_{\mathcal{Z}\in\mathcal{P}^*_K(\mathcal{X})} R(\mathcal{M},\mathcal{Z};D)\big| < \epsilon$

The proof of Proposition 3 is in the Supplementary Material. We give a brief Proof Sketch here. We first identify a class of partitions that we call *"dense partitions"* that satisfy the following property. As the total number of points grows, the density of points in any region should converge to a positive finite value and not to zero. We show that instead of searching among all the partitions it is sufficient to search among the dense partitions. Next, we want to show that if a partition is dense and not ordered, then the loss function can always be improved by making it ordered. To show this, we need to keep a track of the change in the loss function as we move from an unordered to an ordered partition. This is non-trivial to do because the loss function is general and the solution to (4) for a fixed partition does not have a closed form. To track this change, we use *influence functions* [7] and show that the sign of change is always non-positive.

We have now demonstrated that the output of Algorithm 1 and 2 approximately minimize the emprirical risk defined in (4). In the Supplementary Material we show that the hypothesis space represented by the piecewise constant/linear family, which consists of infinite elements, can be approximated with a finite hypothesis class. Next, we use results on PAC learning in Shalev-Shwartz and Ben-David (2014) to prove Theorem 2.

6 Extensions

6.1 Constraint on the shape of the regions:

In the previous section, we developed a method to partition $\mathcal{X}$. However, the subsets forming the partition $\mathcal{Z}$ such as Z_j might be hard to characterize. For instance Z_j may not be a hypercube or even a polyhedron. We add a constraint to the optimization problem to ensure that each of the regions in the partition is easier to characterize.

We require that for each region Z_i all the points in that region are closer to the centroid of Z_i than to the centroid of any other region. Adding such a constraint ensures that each region in the partition is easily described in terms of the centroids. Moreover, it also ensures that each region is a polyhedron.

Suppose data point $x_i \in Z_j$. Let the centroid of the region j is denoted as μ_{Z_j}, where $\mu_{Z_j} = \frac{1}{|Z_j|}\sum_{x_k \in Z_j} x_k$.

$\|x_i - \mu_{Z_j}\| \leq \|x_i - \mu_{Z_k}\|$, $\forall k \neq j$. We add this constraint as a penalty term to the empirical risk defined in (3). The penalized expression for the risk is given as

$$R(\mathcal{M},\mathcal{Z};D) + \sum_{j,k} \lambda \sum_{x_i \in Z_j} \left(\|x_i - \mu_{Z_j}\| - \|x_i - \mu_{Z_k}\|\right)$$

where λ is the price of not satisfying the constraint. We can modify the Algorithm 1 and 2 to incorporate the penalty terms (See details in the Supplementary Material). We can also show that Theorem 1 and 2 can be adapted to this setting provided the space of the partitions is restricted to ordered partitions (See the details in the Supplementary Material). We provide Numerical Results corresponding to this setting in the Supplementary Materials. We provide a summary of all the results in Table 1.

7 Results

7.1 Performance comparison

In this section, we describe the numerical results from experiments using both synthetic and real datasets.

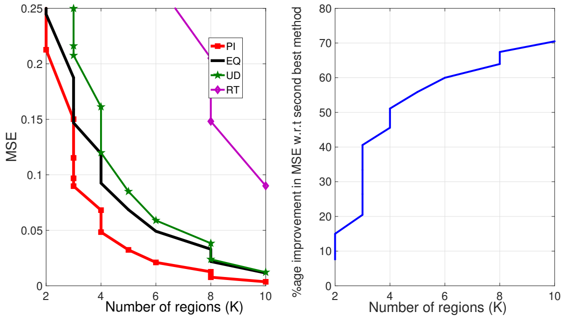
Table 2: Comparison of PI with benchmarks in terms of MSE for piecewise constant models. Black box model: Neural Network

	Synthetic		**Pollution**		**Maggic**		**Wine**	
Algorithm	In	Out	In	Out	In	Out	In	Out
PI	**5**	**11**	**12**	**21**	**8**	**18**	**4**	**8**
EQ	19	32	30	31	30	48	8	17
UD	24	25	40	44	30	35	15	15
RT	196	259	126	131	130	210	34	48

Table 3: Comparison of PI with benchmarks in terms of MSE for piecewise linear models. Black box model: Neural Network

	Synthetic		**Pollution**		**Maggic**		**Wine**	
Algorithm	In	Out	In	Out	In	Out	In	Out
PI-L	**1**	**15**	5	30	**1.9**	**26**	**5.7**	**40**
EQ-L	5	19	20	30	8	31	7.3	42
UD-L	4	18	**0.21**	**27**	6.4	570	11	120
RT	196	259	126	131	130	210	34	48

Figure 2: MSE as a function of the number of regions



We carry out two types of comparisons: one using constant local models and the other using linear local models. We refer to our approach as the piecewise interpreter PI when we use constant local models and PI-L when we use linear local models. The experiments were conducted in Python.

Benchmarks for piecewise constant models: Three natural approaches to partitioning are described next. **Equal Quantiles (EQ)** Divide the feature space (the PSA levels) into K intervals so that the K corresponding populations are equal. **Uniform Division (UD)** Divide the label space (the range of risk values) into K intervals of equal length and partition the feature space (the PSA levels) into the corresponding intervals. **Regression Tree (RT)** Use the predictive model f to construct a regression tree that approximates f with K leaves.

Benchmarks for piecewise linear models If we use linear models inside each region, then we also need to change the benchmarks for fair comparisons. LIME Ribeiro et al. (2016) is a natural competitor for local linear models. However, LIME does not provide a way to partition the feature space. Therefore, we use the above approaches UD and EQ to partition the feature space and then within each cluster that is identified we use LIME to learn a local model. We compare with the combination of UD with LIME (EQ with LIME) which we refer to as UD-L (EQ-L).

Performance metric and comparisons We carry out both in sample and out of sample comparisons. We use mean squared error (MSE) as the loss. For every dataset, we do five-fold cross-validation (80 percent data for training and 20 percent data for testing). In the following comparisons, we set $K = 10$ (a maximum of ten clusters is allowed). In addition, we make sure that all the methods use the same number of clusters so that we have fair comparisons. Also, since the complexity of the method is cubic in the size of the dataset, we use uniform sampling with a rate of 20 samples per iteration. This procedure works for our largest dataset with around 40,000 patients and 30 feature dimensions.

Black Box Models We use two black box models: a feedforward fully connected neural network (NN) (3 layers and 200 nodes per layer) and Random Forest Regression (10 trees, tree depth is 20).

Datasets. We use one synthetic dataset and three real datasets. Two of the real datasets are public datasets from UCI repository. The third dataset is the mortality prediction dataset (Maggic dataset) from Pocock et al. (2012). The details of the datasets are in the Supplementary Materials.

Comparisons For every dataset (synthetic and real), we first learn the black box models above and then compare the performance of our PI with that of other approaches, being careful to compare piecewise constant interpretations with piecewise constant interpretations and piecewise linear interpretations with piecewise linear interpretations. Tables 2,3, show the comparisons for the NN model; the comparisons for the RF model are similar and are shown in the Supplementary Materials. Table 2 shows the comparisons for piecewise constant interpreters; Table 3 shows the comparisons for piecewise linear interpreters. In both tables, we see that in most settings our approach performs much better than other methods (both in and out of sample).

In Table 2,3, we compared the MSE between the interpretive model's prediction and the black box. In the Supplementary Material, we show the MSE between the gradient of a piecewise linear model and the gradient of the black-box model. In the Supplementary Material, we also show the performance of the PI under the additional shape constraints.

Impact of choice of number of regions K: In Figure 2, we compare the performance of the proposed method with other approaches by varying the maximum number of regions from 2-10. Again, our approach consistently outperforms other methods regardless of the choice of K. (Note that regression trees perform poorly because they do not search in the space of ordered partitions.)

7.2 Use case

In this section, we provide a real use case to show that the proposed algorithm, the piecewise interpreter (PI), can be more useful than existing interpreters such as LIME [5]. The use case is based on a medical dataset (Maggic dataset). We use an exemplary patient (features descibed in the Supplementary Material) for comparing LIME with PI. We trained a random forest model (10 trees with a depth of 20).

Performance: For the rest of the comparisons, we use mean squared error (MSE) as the loss function l. The MSE of LIME for the exemplary patient is 0.05. The MSE for PI for the same patient is 0.001. Here we only compare the MSE for one patient. Later we discuss the comparison across all the patients.

Feature rankings and weights by LIME vs PI: The PI finds that the black box assigns a substantially higher weight to BBC (not on Beta Blocker), NYHA (New York Heart Association categories of heart failure), SMK (Smoking), SBC (Shortness of Breath Combined), PCI (Percutaneous Coronary Intervention) in comparison to LIME. In the Supplementary Material, we give the weights assigned by the black box model as computed by the PI and LIME.

Importance of Beta Blocker: As mentioned above we found a stark difference between the importance of the beta blocker as predicted by LIME in comparison to PI for the exemplar patient. We found a group of similar patients (13,000) for which the the magnitude of the weight assigned to beta blocker by LIME as opposed to PI is much smaller. Also, for these patients the average MSE of the PI (0.046) is lesser than the MSE of LIME (0.074). This example shows that the LIME interpreter incorrectly assigns a lower weight to the beta blocker. If the weight of the beta blocker is increased in LIME interpreter, then the MSE reduces. In summary, using an interpreter with a higher MSE can mislead a clinician to believe that the model assigns a lower weight to the beta blockers thus creating mistrust since beta blockers are well known to assist the heart function Doughty et al. (1997).

7.3 Phenotypes

In the previous subsection, we described examples of patients and compared LIME and PI in terms of the feature importance. In this subsection, we compare some of the phenotypes that are computed by the PI for the Maggic dataset. The complete tables describing the phenotypes are in Supplementary Material. Phenotype 2 consists of patients who have poor circulatory systems (exemplified by a low ejection fraction) but normal renal function; for these patients, the most predictive features are blood pressure, myocardial infarction, and diabetes, which are related to circulatory problems. Phenotyope 8 consists of patients who have poor circulatory function and poor renal function; for these patients, the most predictive features are creatinine, hypertension, and blood pressure, which are related to both the renal and circulatory systems. As we can see from this example, an understanding of the most discriminative and most predictive features for each phenotype can help the clinician to better understand both the "how" and the "why" of the predictions of the underlying model.

8 Conclusion

This paper provides a novel way to construct piecewise approximations of a black box model. Our approach uses dynamic programming to partition the feature space into regions and then assigns a simple local model within each region. When we require the local models to be constant (linear) on each cluster, our piecewise approximation is optimal, i.e. it achieves the minimum loss, where the loss measures the distance between the approximation (gradient of the approximation) and the actual prediction (gradient of the prediction). We carry out experiments show that the proposed approach achieves a smaller loss and better reflects the black box model compared to other approaches.

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