

Enhancing Decision Tree based Interpretation of Deep Neural Networks through L1-Orthogonal Regularization^{*}

Nina Schaaf¹ and Marco F. Huber^{1,2}

¹ Fraunhofer IPA, Center for Cyber Cognitive Intelligence CCI, Stuttgart, Germany
nina.schaaf@ipa.fraunhofer.de

² University Stuttgart, Institute of Industrial Manufacturing and Management IFF,
 Stuttgart, Germany
marco.huber@ieee.org

Abstract. One obstacle that so far prevents the introduction of machine learning models primarily in critical areas is the lack of explainability. In this work, a practicable approach of gaining explainability of deep artificial neural networks (NN) using an interpretable surrogate model based on decision trees is presented. Simply fitting a decision tree to a trained NN usually leads to unsatisfactory results in terms of accuracy and fidelity. Using L₁-orthogonal regularization during training, however, preserves the accuracy of the NN, while it can be closely approximated by small decision trees. Tests with different data sets confirm that L₁-orthogonal regularization yields models of lower complexity and at the same time higher fidelity compared to other regularizers.

Keywords: Explainable Artificial Intelligence · Rule extraction from Neural Networks · Regularization · Decision Trees.

1 Introduction

In the recent years, machine learning (ML) gained an increasing interest in a multitude of domains like manufacturing, health care or finance. Deep learning approaches trained on large data sets are already able to compete with and even outperform humans in decision making in some applications like games³ or medical science⁴. Many ML models are considered as “black box”, i.e., decisions made are often not comprehensible to humans due to complex internal processes. It is this complexity, however, that makes modern ML algorithms so powerful—they find patterns in large, high-dimensional data sets that no human could ever discover and the lack of comprehensibility is perfectly sufficient for some applications like movie recommendation or machine translation. For many use cases, however, there is an interest in making black-boxes transparent.

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³ <https://deepmind.com/research/alphago/>, last accessed 23 Mar 2019

⁴ <https://cs.stanford.edu/people/esteva/nature/>, last accessed 28 Mar 2019

One way to enforce so-called *explainability* of ML models is to create models for which the explainability objective is an essential part of their design. *Ante-hoc* models are designed to be inherently explainable; examples for this type of models are logistic regression, rule-based systems [19], or decision trees. In contrast, *post-hoc* explainability refers to adding the explainability objective after training [16,23]. Furthermore, model explainability techniques can either be applicable to a specific model type (*model-specific*) or to a variety of different models (*model-agnostic*). When searching for a suited approach, one has to additionally define the scope of the generated explanations. *Global* explainability—sometimes also called model explainability—implies understanding the model as a whole. In contrast, *local* or output explainability entails knowing the reasons for a specific prediction (or a group of predictions) rather than examining the entire model [14].

Depending on the desired goal, information on the inner workings of ML models can be represented in various ways, for example using visual representations such as heat-maps [5] or plots [11]. Another possibility towards providing explainability is rule extraction from black-box models [13,15,23]. Rule extraction techniques for NNs follow the idea of deriving simple human comprehensible rules from NNs in order to approximate the network’s decision-making process and hence provide explanation capability. Information extracted from NNs can be represented in different formats such as decision trees, decision tables or simple rules of the form:

If weather=sunny and windspeed=low then play tennis

In this paper simple but deep NNs named multi-layer perceptrons (MLP) are considered. A number of works have been published that focus on rule extraction from MLPs. For example, DeepRED [23] uses decision trees as an instrument to extract rules from deep MLPs at the level of the networks’ individual neurons. RxREN [4] prunes insignificant input neurons from a trained MLP and identifies data ranges for the remaining input neurons for rule extraction.

Instead of touching the inner structure of a trained MLP in a post-hoc fashion, the focus in this paper is on *optimizing* deep MLPs towards post-hoc decision tree extraction. For this purpose, a combination of L_1 and orthogonal regularization is proposed, which favors MLPs with decision boundaries that can be approximated much easier by small decision trees. These models allow explainability on a *global* level. By means of numerical evaluation on various public benchmark datasets it is shown that the L_1 -orthogonal regularization approach yields MLPs that maintain a high accuracy, while the extracted decision trees achieve a high fidelity, i.e., they approximate the MLPs well and thus, provide consistent, meaningful, and human comprehensible explanations for deep models.

2 Problem Statement

In this paper multiclass classification is considered, where training is performed by means of a labeled data set $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N$ comprising N samples, where

$\underline{x}_n \in \mathbb{R}^d$ is the input vector of the n -th sample and $y_n \in \mathbb{N}$ is the corresponding label. The elements of \underline{x}_n are named features or attributes.

Multi-layer Perceptron (MLP) To learn the (unknown) mapping from input \underline{x} to output y , an MLP is employed, which consists of multiple neurons that are arranged in two or more layers. These neurons are linked via weighted connections, where the weights of connections from the neurons in layer $l - 1$ to those in layer l are stored in a weight matrix \mathbf{W}_l , with $l \in \{1, \dots, L\}$. In the following, $\mathcal{W} = \{\mathbf{W}_l\}_{l=1}^L$ is the collection of all weight matrices. A column \underline{w}_i of a weight matrix \mathbf{W}_l comprises the weights of connections from all neurons of layer $l - 1$ to the i -th neuron of layer l .

An MLP's output \hat{y}_n is computed via a function $f(\underline{x}_n, \mathcal{W})$. MLP training aims for adjusting the weights in \mathcal{W} by means of solving the optimization problem

$$\min_{\mathcal{W}} \sum_{n=1}^N E(y_n, f(\underline{x}_n, \mathcal{W})) + \lambda \cdot \Omega(\mathcal{W}) \quad (1)$$

such that the error E between the MLP's outputs \hat{y}_n and the given targets y_n is minimized. In (1), $\Omega(\mathcal{W})$ is a so-called *regularization term*, whose strength can be controlled by a regularization parameter $\lambda \in \mathbb{R}$. Usually, this term is used to avoid overfitting.

Decision Trees (DT) In this paper, DTs are used for extracting explanations from a trained MLP. A DT consists of internal and leaf nodes. The internal nodes specify tests of the value of one of the input attributes whereas the leaf nodes specify class labels [17]. To classify an example, the tree is traversed from top to bottom. If an internal node is reached and the test is passed, the left path, otherwise the right one is followed. This procedure is repeated at each of the following internal nodes until a leaf node is reached. Every path from the tree's root to a leaf node can be translated into a if-then-rule like the one shown above. The condition of the if-clause then corresponds to the tests along the path.

Related Work on DT Extraction In Alg. 1, a meta-algorithm for DT extraction from a trained MLP is shown. Here, the MLP is considered as an oracle that is fed with various inputs \underline{x} to predict outputs y . This data is then used to learn a DT. A naïve way is to use no regularization, i.e., $\Omega = 0$. In [8] this approach was extended by considering the data distribution and constraints when sampling the inputs, but MLP training is not influenced to improve the accuracy of the extracted DT.

Wu et al. [20] instead present a novel regularizer called *tree regularization*, where Ω represents the *average-path-length* (APL) cost function. The idea is to train an MLP in such a way that the extracted DT are rather shallow. Unfortunately, APL cannot be calculated in closed-form: a DT needs to be trained first in order to calculate the APL. Thus, APL is also not differentiable, which

Algorithm 1 MLP training and subsequent DT extraction. Given a labeled data set \mathcal{D} and regularizer Ω , the MLP is trained by solving (1) together with an appropriate loss function E . The resulting weight matrices \mathcal{W} and the training data $\{\underline{x}_n\}_{n=1}^N$ are used to generate predictions \hat{y}_n from the MLP. Finally, the DT is trained with $\{\underline{x}_n, \hat{y}_n\}_{n=1}^N$.

Input: $\mathcal{D} = \{\underline{x}_n, y_n\}_{n=1}^N$: data set with N examples. $\Omega(\cdot)$: regularization term
function TRAINANDEXTRACTDT:
 $\mathcal{W} \leftarrow \text{TRAINMLP}(\mathcal{D}, \Omega)$
 $\{\hat{y}_n\} \leftarrow f(\{\underline{x}_n\}, \mathcal{W})$
 $\text{tree} \leftarrow \text{TRAINDT}(\{\underline{x}_n, \hat{y}_n\})$
return \mathcal{W} , tree

complicates MLP training in addition. To overcome these issues, [20] propose to learn an additional surrogate MLP for estimating the APL. It is obvious that simultaneously training two interrelated MLPs requires significant training time and careful parameter tuning.

3 L1-Orthogonal Regularization

The goal is to avoid the limitations of tree regularization but at the same time maintain its appealing idea. For this purpose a closed-form, simple to implement, and differentiable regularization is proposed that forces the decision boundaries of the trained MLP to be easily approximated by a DT. In addition, the trained MLP should result in a DT with shorter path lengths than a DT extracted from an MLP trained without or with other regularizers. However, the MLP's predictive accuracy should not decrease significantly when applying the regularizer during training. In order to achieve this goal, we propose promoting both sparseness and orthogonality of the weight vectors \underline{w} in the weight matrices \mathbf{W} .

It is well known that a weight vector represents the normal vector of linear decision boundary. By means of enforcing a sparse representation, where many or even all but one elements of a weight vector are close to zero, the linear decision boundary becomes axis parallel. This representation is likely to harmonize well with DTs. It can be shown that the decision boundary of a DT consists of axis-parallel segments, as each test node in a DT divides the input space into axis-aligned hyperplanes, where each hyperplane is labeled with one class.

Further, we want to avoid that too many decision boundaries are (almost) parallel to each other, i.e., many weight vectors point into a similar direction. This would limit the predictive power of the model and thus, sparseness is combined with orthogonality, i.e., the weight vectors are encouraged to be close to orthogonal in a pair-wise fashion. By combining sparse with orthogonal regularization during MLP training it is intended that a weight matrix \mathbf{W} contains a small number of non-zero entries (sparse) that nevertheless cover a broad spectrum of features (orthogonal). This kind of regularization drives MLPs to have

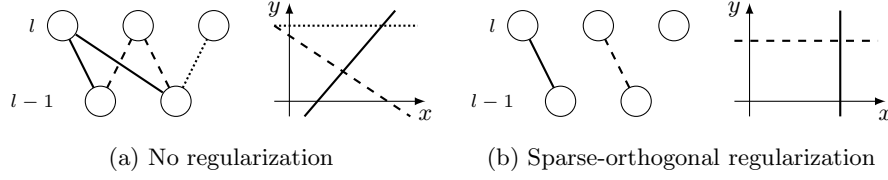


Fig. 1: Effect of sparse-orthogonal regularization on an MLP's weight vectors.

decision boundaries being more similar to those of DTs and thus, can be better approximated.

Figure 1 shows the intended effects on weight vector alignment when applying the proposed sparse-orthogonal regularization approach. Here, the weights between two consecutive layers are schematically illustrated. The weights on the connections of all neurons of layer $l-1$ to a neuron of layer l form the elements of the weight vector. No connection means that the corresponding weight is equal to zero. If a neuron in layer l has more than one connection, the weight vector is not axis parallel as can be seen in Fig. 1a. The network in Fig. 1b instead is both sparse (few connections) and has orthogonal weight vectors (connections to different neurons in layer $l-1$).

3.1 Regularizers

In the following, different regularization terms are introduced for inducing sparsity and orthogonality into an MLP for tree extraction.

L1 Regularization Ideally, one should apply the L_0 -norm in order to obtain maximum sparsity, i.e., all elements of a column vector \underline{w} of \mathcal{W} are exactly zero except of one. This approach, however, is not feasible in practice, as the L_0 -norm is known to be non-differentiable. Instead, an approximation to the L_0 -norm is required. A well known approximation is the L_1 -norm

$$\Omega_1(\mathcal{W}) = \sum_l \|\mathbf{W}_l\|_1, \quad (2)$$

where $\|\mathbf{A}\|_1 = \sum_i |\underline{a}_i| = \sum_i \sum_j |a_{ij}|$ is the so-called *1-Norm* of matrix \mathbf{A} , with \underline{a}_i being the i -th column vector of \mathbf{A} .

Orthogonal Regularization The aim of orthogonal regularization is to orthogonally align the weight vectors \underline{w}_i in each layer of an MLP. Xie et al. [21] propose the following method to promote orthogonality: Two vectors \underline{w}_i and \underline{w}_j are orthogonal if their inner product $\underline{w}_i^T \underline{w}_j$ is zero and their L_2 -norms $\|\underline{w}_i\|_2$ and $\|\underline{w}_j\|_2$ are close to one. For simultaneously promoting orthogonality between all pairs of weight vectors of \mathbf{W} , one can consider the corresponding Gram matrix $\mathbf{G}_{ij} = \underline{w}_i^T \underline{w}_j$. The Gram matrix consists of the pair-wise scalar products of the weight matrix' columns, where the Gram matrix' diagonal elements (the Gram

determinant) are $\|\underline{w}_i\|_2$ [2]. Encouraging \mathbf{G} to be close to the identity matrix \mathbf{I} makes $\underline{w}_i^T \underline{w}_j$ close to zero and $\|\underline{w}_i\|_2$ close to one, resulting in near-orthogonality of the weight vectors [22].

To compute the scalar product of all weight vectors of a layer's weight matrix \mathbf{W}_l one can simply compute the Gram matrix $\mathbf{G}_l = \mathbf{W}_l^T \mathbf{W}_l$. Thus, near-orthogonality among the weight vectors in each layer l can be promoted by substituting Ω in (1) with the regularization term

$$\Omega_{\text{orth}}(\mathcal{W}) = \sum_l \|\mathbf{G}_l - \mathbf{I}\|_1. \quad (3)$$

Here, $\|\cdot\|_1$ is the 1-Norm as in (2).

Alternatives As with vectors, there are several options to compute the norm of matrices. One alternative approach of measuring the closeness between \mathbf{G} and \mathbf{I} is using the so-called *Frobenius norm* (FN)

$$\|\mathbf{A}\|_F^2 = \sqrt{\sum_i \sum_j |a_{ij}|^2} \quad (4)$$

as described in [21]. Experimental evaluations indicate (see Sec. 5 for details) that both norms often provide similar results, with slight advantages for the 1-Norm. Also from a numerical perspective, the 1-Norm turned out to be more reliable and thus, we recommend to use the 1-Norm.

A further alternative is the so-called log-determinant divergence (LDD) for measuring the closeness between \mathbf{G} and \mathbf{I} by encouraging their LDD

$$\Omega_{\text{LDD}}(\mathcal{W}) = \text{tr}(\mathbf{G}) - \log \det(\mathbf{G}) \quad (5)$$

to be small [22], where $\text{tr}(\cdot)$ is the matrix trace and $\det(\cdot)$ is the matrix determinant.

However, applying (5) to gradient descent optimization leads to the following problem. For $f(\mathbf{A}) = \log \det \mathbf{A}$, the gradient is defined as $\nabla f(\mathbf{A}) = \mathbf{A}^{-T}$ [6]. Inverting \mathbf{A} , however, is difficult to impossible when \mathbf{A} is close to be singular. Consequently, numerical errors occur during training when the Gram matrix's determinant approaches zero.

L_1 -Orthogonal (L_1 -O) Regularization Based on the aforementioned discussions, L_1 regularization (2) and orthogonal regularization based on the 1-Norm (3) are combined to form *L_1 -orthogonal* (L_1 -O) regularization

$$\Omega(\mathcal{W}) = \lambda_1 \cdot \Omega_1(\mathcal{W}) + \lambda_{\text{orth}} \cdot \Omega_{\text{orth}}(\mathcal{W}) \quad (6)$$

to be employed in (1). But instead of a single regularization parameter λ as in (1), the regularization strengths of Ω_1 and Ω_{orth} are regulated independently via λ_1 and λ_{orth} , respectively. With the independent parameterization of the regularization strengths, both regularizers and their trade-offs can be individually controlled, which turned out to be highly beneficial during empirical investigations.

3.2 Remark

It is worth mentioning that L₁ is not new to NN training and also the combination of sparseness and orthogonality has already been proposed (see e.g., [21]). In contrast to [21], the regularization combination proposed in this paper is numerically by far more stable as inverting singular weight matrices is avoided. But more important, to the best of our knowledge, this is the first time that sparse-orthogonal regularization has been proposed and investigated for the purpose of extracting explainable ML models from deep NNs.

4 Experiments

To evaluate the L₁-O regularization approach, detailed experiments are performed on simulated and real-world data sets. For this purpose, L₁-O regularization’s performance is compared with three alternative regularizers: L₁, orthogonal and tree regularization. Additionally, as a baseline, a standalone DT classifier, i.e., a DT directly trained on the data, and an MLP without regularization are considered.

In order to additionally compare the effect of the matrix norm used to enforce orthogonality, the regularizers (3) and (4) are evaluated as well and are abbreviated 1-Norm and FN, respectively, in the following.

4.1 Evaluation Criteria

In 1995, Andrews et al. [3] introduced a taxonomy consisting of five criteria for categorizing rule extraction techniques. For the evaluation, the fourth and the fifth criterion, namely the *quality* of the rules and the *complexity* of the rule extraction technique itself are of interest. Andrews et al. define the four quality measures for rules: (1) accuracy, (2) fidelity, (3) consistency, and (4) comprehensibility. The evaluation measures listed below are mainly based on these criteria.

Complexity vs. predictive performance Complexity of a DT is measured by the APL metric, i.e., the average number of decision nodes that must be passed to make a prediction, proposed in [20]. The predictive performance of the corresponding MLP is measured by the area under the ROC curve (AUC).

APL reduction With the APL reduction metric the effect of regularization on the DT’s complexity is measured. For this purpose, the APL of DTs extracted from a regularized MLPs is compared to an DT extracted from an unregularized MLP. This metric has two characteristics: (1) maximum achieved APL reduction (APL_{max}) and (2) APL reduction of a DT with the same or better predictive performance than the DT extracted from an unregularized network (APL_{com}). Both APL metrics are normalized according to $\frac{APL_{\star} - APL_{base}}{APL_{base}} \times 100$, where $\star \in \{\text{max, com}\}$ and APL_{base} is the average path length of the DT extracted from an unregularized MLP.

Fidelity This criterion quantifies how well the DT mimics the behavior of the MLP from which it was extracted [3]. Fidelity is defined as the percentage of test examples on which the prediction made by a DT agrees with the prediction of the MLP [8], i.e.,

$$\text{Fidelity} = 1 - \text{Prob}\{\underline{x} \in \mathcal{T} | f_{\text{DT}}(\underline{x}) \neq f_{\text{N}}(\underline{x})\}, \quad (7)$$

where \mathcal{T} is the test set and $f_{\text{DT}}(x)$, $f_{\text{N}}(x)$ are the functions implemented by the DT and MLP, respectively. The higher the fidelity, the better the DT reflects the MLP and the more reliable are the conclusions drawn from it.

Comprehensibility Complexity vs. predictive performance measures how reduction in model complexity (measured by the APL) effects the predictive performance. The intention behind the comprehensibility criterion is to evaluate the DTs’ comprehensibility by visually examining the trees themselves.

Consistency Andrews et al. [3] define that consistency is given if the rules extracted under different training sessions produce the same classifications of test examples. Consistency is defined as

$$\text{Consistency} = 1 - \text{Prob}\{\underline{x} \in \mathcal{T} | f_{\text{DT}_1}(\underline{x}) = f_{\text{DT}_2}(\underline{x}) = \dots = f_{\text{DT}_S}(\underline{x})\}, \quad (8)$$

where $f_{\text{DT}_i}(\underline{x})$ is the function implemented by the DT extracted from the MLP in training session $i \in \{1, \dots, S\}$. In addition, the generated DTs should be as similar as possible (visual inspection).

Computational complexity The computation times of L_1 -O and tree regularization are compared, in order to assess computational efficiency of the less complex L_1 -O regularization.

4.2 Data Sets and Networks

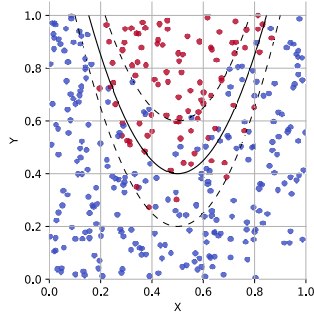


Fig. 2: Training data and class labels for 2D-parabola problem.

Toy Data Set For a first comparison of the different regularizers, the 2D-parabola problem introduced in [20] is chosen. As shown in Fig 2, the training data consists of 2D input points whose two-class decision boundary is roughly shaped like a parabola and is defined by $y = 5 \cdot (x - 0.5)^2 + 0.4$. For data generation, 500 points are sampled uniformly within a box of size $[0, 1] \times [0, 1]$. Those points lying above the decision boundary are labeled positive. Finally, 10% of the points near the boundary (limited by $y = 5 \cdot (x - 0.5)^2 + 0.2$ and $y = 5 \cdot (x - 0.5)^2 + 0.6$, plotted as dashed lines in Fig. 2) are flipped.

The MLP trained on the parabola data comprises three hidden layers with 100, 100, and 10 neurons, respectively. The tree regularization’s surrogate MLP has one hidden layer with 25 nodes. The main MLP applies ReLU activation in the hidden layers and sigmoid activation in the output layer while the surrogate MLP applies Tanh activation in the hidden layer and softplus activation in the output layer. The objective in (1) is optimized via Adam gradient descent [12].

Table 1: Data sets and MLPs used for evaluation.

| Data set | #instances | #features | #classes | #neurons |
|-----------------------------|------------|-----------|----------|----------|
| Iris [10] | 150 | 4 | 3 | 10 |
| Breast Cancer Wisconsin [9] | 569 | 30 | 2 | 25 |
| Pima Indians Diabetes [9] | 768 | 8 | 2 | 32, 16 |
| Titanic [1] | 1,309 | 11 | 2 | 30 |
| Mushroom [9] | 8,124 | 22 | 2 | 32 |
| Adult [9] | 48,842 | 14 | 2 | 32, 16 |
| Diabetes [18] | 100,000 | 50 | 2 | 100, 10 |

Real-World Data Sets The 2D-parabola problem was chosen to compare L₁-O regularization’s performance to tree regularization on a simple data set. Additional, further experiments with more complex data sets were performed. These data sets cover different sizes (150–100,000) and varying numbers of features (4–50). With these data sets, both shallow and deep MLPs were trained—deep MLPs are defined as networks comprising more than one hidden layer.

Table 1 summarizes the data sets and sizes of the hidden layers of the MLPs used for the experiments. *Iris* is a multi-class data set and distinguishes three iris plants. *Breast Cancer Wisconsin (Diagnostic)* data set contains information on cell nuclei that are used to determine whether cancer is malignant or benign, while with the *Pima Indians Diabetes* data set one can investigate whether a patient shows signs of diabetes. The *Titanic* data set contains information on passengers of the Titanic and whether they survived the sinking of the ship. The *Mushroom* data set describes mushrooms in terms of physical characteristics and distinguishes between poisonous and edible mushrooms. Using the *Adult* data set, that contains census data, the prediction task is to determine whether a person’s income exceeds US\$ 50,000 per year. *Diabetes* data set represents clinical care at 130 US hospitals and integrated delivery networks during 1999–2008 and is used to predict whether a patient gets readmitted to hospital.

The MLPs listed in Table 1 apply ReLU activation in the hidden layers and sigmoid and softmax activation in the output layer for binary and multi-class classification, respectively. The MLPs’ objective was optimized via Adam gradient descent [12]. Hyperparameters (layer sizes, batch size, epochs, learning rate) were set via 3-fold cross validation (CV) using grid search. For tree regularization the same architecture for the surrogate MLP as with the toy data is used.

4.3 Training

For MLP training, each data set is split into subsets for training (70%) and testing (30%). Afterwards, a grid search is carried out using a wide range of regularization parameters for each regularization type. In doing so, it is possible to cover as many decision boundary complexities as possible for each technique. All weights are initialized using the same random seed. For the two large data sets Adult and Diabetes, the DTs are trained with a fixed `minimum-samples-leaf` parameter that defines the minimum number of samples required to be at a

leaf node [7]. This parameter allows a reduction in the number of branches and generation of a smoother tree with a lower APL. Without limiting the number of samples at a leaf node, the path lengths of the generated trees are between 1,000 and 10,000 and thus, incomprehensible. All experiments are conducted on a single Intel Core i7 CPU on Windows 7.

Since training tree-regularized MLP’s turned out to be problematic, it is only possible to provide results for 2D-parabola, Iris, and Breast Cancer data sets. One explanation for the challenging training process could be the high amount of free parameters (for the main MLP as well as the surrogate MLP), which leads to a wide spectrum of potential error sources.

5 Discussion

Complexity vs. predictive performance In Fig. 3, MLP complexity is plotted against predictive performance for a selection of MLPs—each trained with different regularization strengths being displayed as single points in a 2D fitness space. Additionally, the AUC of an unregularized MLP is illustrated as black dotted line in order to provide a baseline.

For the 2D-parabola data set, L_1 regularization does not produce DTs with both small node counts and good predictions. In contrast, the DTs resulting from orthogonal and L_1 -O regularization are of reduced complexity—with a relatively low predictive accuracy, though. The only approach that produces highly accurate results with an at the same time small APL is tree regularization. However, comparing tree regularization and L_1 -O regularization on the Iris data set already shows, that L_1 -O regularization can compete with tree regularization. Both regularizers encourage simple and accurate models.

When looking at the fitness curves of the remaining real-world data sets, it can be noticed that L_1 -O regularization consistently outperforms the other regularizers. The differences between L_1 regularization, standalone DTs and L_1 -O regularization are relatively small for some data sets (cf. Iris, Titanic), while for other data sets, L_1 -O regularization achieves much higher reductions in complexity than standalone DTs and L_1 regularization (cf. Pima Indians Diabetes, Adult, Diabetes). With orthogonal regularization alone, for non of the real-world data sets a significant reduction in model complexity can be achieved.

In summary, it can be said, that L_1 -O regularization’s performance on the 2D-parabola data set is relatively poor, while on the other data sets the approach convinces with *simple and accurate* models. This can be explained by the concept behind this approach. With L_1 -O regularization, MLPs with few connections that nevertheless cover a broad spectrum of features due to their orthogonal alignment can be learned. Since the 2D-parabola data set contains only two input attributes, the variety of feature combinations is limited. The other data sets contain more input attributes providing more combinatorial options that can be exploited.

Furthermore, the results show that it is the *combination* of L_1 and orthogonal regularization that makes this regularizer powerful. Applying L_1 -O regulariza-

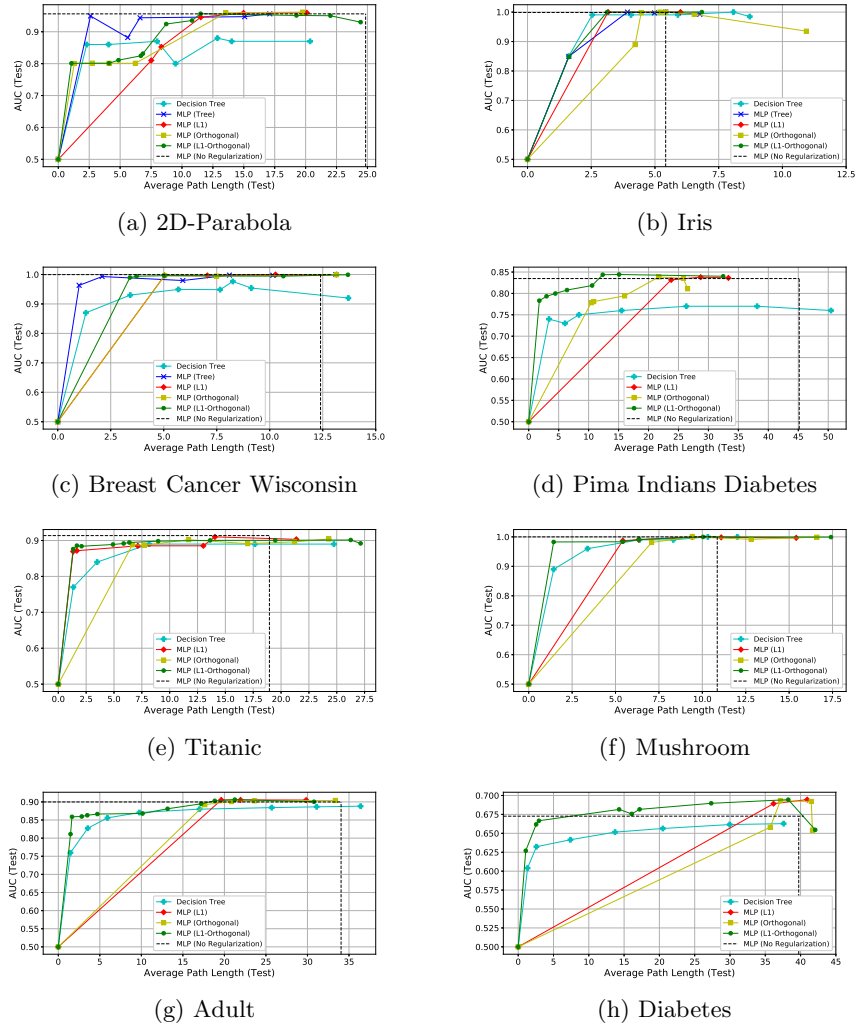


Fig. 3: Fitness curves showing prediction quality (AUC) vs. complexity (APL).

tion leads to significantly better results than applying L₁ regularization and orthogonal regularization alone.

APL reduction In order to measure APL reduction, at first the MLPs that meet APL_{max} and APL_{com} are determined via a grid search over regularization parameters. Next, for each data set 5-fold CV is performed, with the regularization parameters identified before being fixed. Table 2 lists the means and standard deviations for both APL reduction values.

With L₁-O regularization (1-Norm and FN), a significant maximum reduction of the APL is achieved for all data sets. The same holds for the APL of DTs

Table 2: APL reduction according to (a) APL_{\max} and (b) APL_{com} .

| Data set | $L_1\text{-O}$ | | | | L_1 | | Tree | |
|---------------|--------------------------------|--------------------------------|-------------------------------|--------------------------------|-------------------------------|--------------------------------|--------------|--------------------------------|
| | 1-Norm | | FN | | | | | |
| | (a) | (b) | (a) | (b) | (a) | (b) | (a) | (b) |
| 2D-parabola | -80 ± 7 | $+9 \pm 25$ | -90 ± 4 | -10 ± 15 | -12 ± 28 | -9 ± 15 | -53 ± 23 | -10 ± 11 |
| Iris | -72 ± 3 | -15 ± 17 | -13 ± 8 | -25 ± 23 | -63 ± 51 | -63 ± 51 | $+41 \pm 70$ | $+14 \pm 21$ |
| Breast Cancer | -57 ± 12 | -39 ± 20 | -53 ± 8 | -39 ± 20 | -38 ± 16 | -38 ± 16 | -4 ± 39 | -15 ± 39 |
| Pima Indians | -89 ± 5.1 | -62 ± 11 | -98 ± 1 | -86 ± 10 | -32 ± 5 | -32 ± 5 | - | - |
| Titanic | -91 ± 1 | -46 ± 17 | -94 ± 1 | -28 ± 19 | -84 ± 8 | -17 ± 10 | - | - |
| Mushroom | -87 ± 1 | -31 ± 18 | -87 ± 1 | -20 ± 42 | -87 ± 1 | -43 ± 7 | - | - |
| Adult | -86 ± 5 | -14 ± 9 | -93 ± 4 | -10 ± 11 | -12 ± 25 | -12 ± 25 | - | - |
| Diabetes | -95 ± 1.3 | -74 ± 2 | -99 ± 1 | -86 ± 8 | -55 ± 24 | -55 ± 24 | - | - |

with a predictive quality being comparable to the benchmark DT. Here APL reduction is obtained for all real-world data sets. In some cases the reduction of the path length is immense (cf. Titanic and Diabetes). For the tree regularization approach, APL reductions can be observed for the 2D-parabola and Breast Cancer data set whereas for the Iris data set the APLs increase. With L_1 regularization, reductions could also be achieved, yet in most cases they are lower than or equal (cf. Mushroom) to those of $L_1\text{-O}$ regularization.

At a first glance, the results for sparse-orthogonal regularization with FN seem to be better than sparse-orthogonal regularization with 1-Norm (i.e., $L_1\text{-O}$), but a closer look at the AUC indicates some issues with FN. For instance, for the data sets where APL reduction with FN is very high (e.g., Adult or Diabetes), the mean AUC over all five folds is close to 0.5. This means the extracted DTs are not better than flipping a coin. In contrast, the DTs resulting from $L_1\text{-O}$ regularization are close to the benchmark MLP (recall Fig. 3). In case of the Diabetes data set, the mean AUC values are 0.64 and 0.68 for APL_{\max} and APL_{com} , respectively, and thus, are close to or even better than the AUC value of the unregularized MLP. Hence, $L_1\text{-O}$ regularization (with 1-Norm) produces better results with respect to the predictive performance.

Fidelity For measuring fidelity, first the “best” performing DT from the grid search over regularization parameters is determined, which corresponds to the DT with the smallest APL that reaches the predictive performance of an unregularized MLP. Next, for each data set 5-fold CV is performed with the regularization parameters obtained from the best model being fixed. Table 3 lists the mean fidelity and corresponding standard deviations for DTs extracted from MLPs with $L_1\text{-O}$ (1-Norm and FN), tree, and L_1 regularization as well as from an unregularized MLP for all data sets.

Here, two things can be noticed. First, DTs extracted from regularized MLPs have very high fidelity scores that are mostly in a similar range. Second, regularization in general has a positive impact on fidelity, as with regularization the fidelity improves in most cases while simultaneously the APLs are reduced. This can be observed particularly for Diabetes and Pima Indians Diabetes data sets.

Table 3: Fidelity values of DT predictions.

| Data set | Fidelity | | | | |
|---------------|--------------------|--------------------|--------------------|-------------|--------------------|
| | L ₁ -O | | L1 | Tree | unregularized |
| | 1-Norm | FN | | | |
| 2D-parabola | 0.95 ± 0.00 | 0.96 ± 0.02 | 0.97 ± 0.02 | 0.96 ± 0.01 | 0.96 ± 0.01 |
| Iris | 0.99 ± 0.01 | 0.97 ± 0.02 | 0.99 ± 0.02 | 0.93 ± 0.04 | 0.97 ± 0.03 |
| Breast Cancer | 0.96 ± 0.01 | 0.95 ± 0.02 | 0.95 ± 0.02 | 0.92 ± 0.04 | 0.94 ± 0.02 |
| Pima Indians | 0.94 ± 0.01 | 0.98 ± 0.00 | 0.90 ± 0.04 | - | 0.86 ± 0.02 |
| Titanic | 0.98 ± 0.00 | 0.98 ± 0.01 | 0.97 ± 0.01 | - | 0.96 ± 0.01 |
| Mushroom | 1.00 ± 0.00 | 1.00 ± 0.00 | 1.00 ± 0.00 | - | 1.00 ± 0.00 |
| Adult | 0.95 ± 0.00 | 0.94 ± 0.00 | 0.94 ± 0.00 | - | 0.91 ± 0.01 |
| Diabetes | 0.94 ± 0.00 | 0.98 ± 0.01 | 0.94 ± 0.03 | - | 0.88 ± 0.00 |

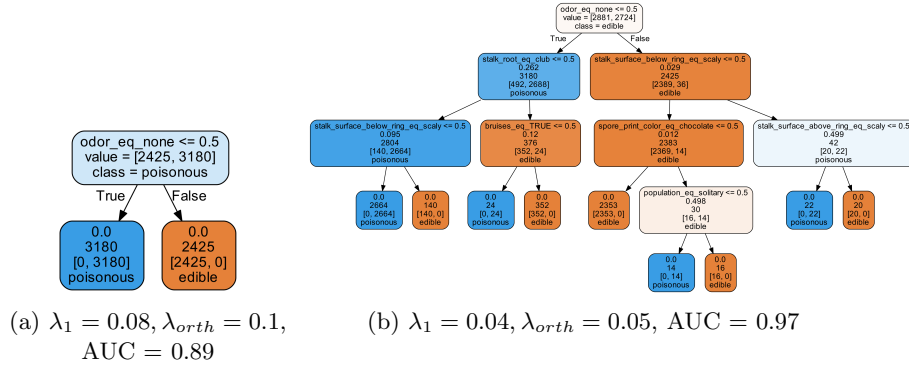


Fig. 4: Small DTs for Mushroom data set.

In general, L₁-O regularization achieves excellent fidelity scores: all scores are ≥ 0.94 . Thus, by analyzing the DTs it is possible to draw reliable conclusions about behavior and decision making of the MLP from which they were extracted.

Comprehensibility Fig. 4a and 4b show two small DTs for the Mushroom data set with an APL of 1 and 6.3, respectively. This comparison demonstrates that an extremely short path length is not necessarily beneficial for the comprehensibility of the DTs. The DT in Fig. 4a classifies instances by only testing on one feature (`odor_eq_none`). Given this little information, it is hardly possible to get insights about the decision making of the MLP. In contrast, the DT shown in Fig. 4b has a higher APL, but nevertheless provides information in a clear and concise manner and enables a more detailed investigation.

This example shows that model complexity and comprehensibility are not necessarily the same. Consequently, when optimizing an MLP with regard to model complexity *and* comprehensibility one has to find a trade-off between the two demands. Although a reduction in model complexity can improve comprehensibility significantly, a model that is too simple is scarcely meaningful.

Table 4: Consistency of DT predictions and similarity of DTs.

| Data set | λ_1 | λ_{orth} | APL | Consistency | Similarity | Fidelity |
|----------|-------------|-------------------------|------|-------------|------------|-----------------|
| Titanic | 0.07 | 0.75 | 1.4 | 1.0 | yes (9/10) | 1.0 ± 0.0 |
| | 0.0075 | 0.75 | 9.7 | 0.94 | no (0/10) | 1.0 ± 0.0 |
| | 0.001 | 0.005 | 19.1 | 0.91 | no (0/10) | 0.98 ± 0.01 |
| | 0.001 | 0.001 | 20.2 | 0.92 | no (0/10) | 0.98 ± 0.01 |
| Mushroom | 0.07 | 0.075 | 1.1 | 0.52 | no (0/10) | 1.0 ± 0.0 |
| | 0.03 | 0.05 | 6.1 | 0.98 | no (0/10) | 1.0 ± 0.0 |
| | 0.03 | 0.025 | 7.1 | 0.99 | no (0/10) | 1.0 ± 0.0 |
| | 0.006 | 0.01 | 21.7 | 0.98 | no (0/10) | 1.0 ± 0.0 |
| Adult | 0.08 | 1.1 | 2.4 | 0.75 | no (3/10) | 0.99 ± 0.01 |
| | 0.07 | 1.5 | 3.8 | 0.79 | no (0/10) | 0.99 ± 0.01 |
| | 0.02 | 0.5 | 16.3 | 0.85 | no (0/10) | 0.96 ± 0.01 |
| | 0.001 | 0.05 | 20.0 | 0.93 | no (0/10) | 0.94 ± 0.00 |
| Diabetes | 0.03 | 0.1 | 2.0 | 0.67 | no (4/10) | 1.0 ± 0.0 |
| | 0.02 | 0.075 | 6.3 | 0.54 | no (0/10) | 0.98 ± 0.01 |
| | 0.008 | 0.05 | 21.2 | 0.81 | no (0/10) | 0.94 ± 0.02 |
| | 0.007 | 0.025 | 21.4 | 0.87 | no (0/10) | 0.92 ± 0.01 |

Consistency To measure consistency of L_1 -O regularization, ten MLPs are trained with fixed regularization parameters and random weight initialization. Afterwards, a DT is extracted from each MLP and is used to classify the test examples for calculating (8). Additionally, the DTs themselves are compared visually for similarities.

Consistency is quantified for four regularization configurations. The results for four data sets are listed in Table 4 in ascending order of the complexity of the generated DTs (APL). There are various interesting observations: (1) The stronger L_1 -O regularization the higher is the fidelity, which is a highly desirable behavior. (2) The lower the model complexity (small APL), the higher DT similarity. This is not surprising as nodes in a DT being near the root are similar but as the trees grow, differences are more likely to occur. However, the different DTs nevertheless agree in classifying test examples. (3) The consistency tends to become lower with a stronger L_1 -O regularization. There are two explanations for this behavior. First, DTs are known to be quite unstable, because each split point depends on the parent split. Thus, if a different feature gets selected as test node, the whole tree changes [14]. Second, MLPs were initialized with random weights and thus, the trained MLPs are all different as (1) is a non-convex optimization problem. L_1 -O regularization seems to be more sensitive to initialization.

Computational complexity As it was not possible to produce satisfying results for tree regularization for all data sets, only the run-times measured for 2D-parabola, Iris, and Breast Cancer data sets can be compared. As Table 5 indicates, the run times of tree-regularized models are 30–70 times higher than those of an L_1 -O-regularized model.

Table 5: Computation time in seconds of L₁-O and tree regularization.

| Regularization | 2D-parabola | Iris | Breast Cancer |
|-------------------|--------------|-------------|---------------|
| L ₁ -O | 42.72 | 0.59 | 6.44 |
| Tree | 2,841.56 | 17.78 | 471.49 |

6 Conclusions and Future Work

In this paper, L₁-O regularization was proposed for improving the extraction of decision trees from deep neural networks. This regularization approach influences the network’s nonlinear decision boundary in such a way that it can be well-approximated by small DTs. These explainable models can provide users of different interest-groups insights into the decision making of the associated network in a representation format that is easily comprehensible. It was shown that the extracted trees mimic the associated networks with high fidelity. Consequently, the conclusions drawn by interpreting the DTs are highly consistent in terms that they reflect the behavior of the associated deep model.

The experiments proved the technical ability of L₁-O regularization to reduce model complexity. However, the inspection of the generated DTs showed that extremely short path lengths do not necessarily have to be favorable for DT comprehensibility. Thus, a next step could be to conduct detailed user studies with different user groups (including domain experts) in order to analyze the extracted DTs with regard to their comprehensibility and supportive potential.

This paper focused exclusively on the extraction of DTs from MLPs. Future work is also devoted to explore the effect of L₁-O regularization on other types of explainable models like decision tables or decision sets. Also applicability of L₁-O regularization for different NN types like recurrent or convolutional NNs needs to be investigated.

References

1. Titanic: Machine Learning from Disaster (2012), <https://www.kaggle.com/c/titanic/data>, last accessed 30 Mar 2019
2. Gram matrix. In: Encyclopedia of Mathematics (2014), https://www.encyclopediaofmath.org/index.php/Gram_matrix
3. Andrews, R., Diederich, J., Tickle, A.B.: Survey and critique of techniques for extracting rules from trained artificial neural networks. Knowledge-Based Systems **8**(6), 373–389 (1995). [https://doi.org/10.1016/0950-7051\(96\)81920-4](https://doi.org/10.1016/0950-7051(96)81920-4)
4. Augasta, M.G., Kathirvalavakumar, T.: Reverse Engineering the Neural Networks for Rule Extraction in Classification Problems. Neural Processing Letters **28**(3) (2011)
5. Bach, S., Binder, A., Montavon, G., Klauschen, F., Müller, K.R., Samek, W.: On Pixel-Wise Explanations for Non-Linear Classifier Decisions by Layer-Wise Relevance Propagation. PloS one **10**(7), e0130140 (2015). <https://doi.org/10.1371/journal.pone.0130140>

6. Boyd, S., Vandenberghe, L.: *Convex Optimization*. Cambridge University Press, New York, NY (2009)
7. Buitinck, L., Louppe, G., Blondel, M., Pedregosa, F., Mueller, A., Grisel, O., Niculae, V., Prettenhofer, P., Gramfort, A., Grobler, J., Layton, R., Vanderplas, J., Joly, A., Holt, B., Varoquaux, G.: API design for machine learning software: experiences from the scikit-learn project. In: *ECML PKDD Workshop: Languages for Data Mining and Machine Learning*. pp. 108–122 (2013)
8. Craven, M.W., Shavlik, J.D.: Extracting tree-structured representations of trained networks. In: *Proceedings of the 8th International Conference on Neural Information Processing Systems (NIPS)*. pp. 24–30 (1996)
9. Dua, D., Graff, C.: *UCI Machine Learning Repository* (2017), <http://archive.ics.uci.edu/ml>
10. Fisher, R.A.: The Use of Multiple Measurements in Taxonomic Problems. In: *Annals of Eugenics*, vol. 7, pp. 179–188 (1936)
11. Friedman, J.H.: Greedy function approximation: A gradient boosting machine. *Ann. Statist.* **29**(5), 1189–1232 (2001). <https://doi.org/10.1214/aos/1013203451>
12. Kingma, D.P., Ba, J.: Adam: A Method for Stochastic Optimization, *arXiv:1412.6980*
13. Lakkaraju, H., Kamar, E., Caruana, R., Leskovec, J.: Interpretable & Explorable Approximations of Black Box Models, *arXiv:1707.01154*
14. Molnar, C.: *Interpretable Machine Learning. A Guide for Making Black Box Models Explainable* (2019), <https://christophm.github.io/interpretable-ml-book/>
15. Puri, N., Gupta, P., Agarwal, P., Verma, S., Krishnamurthy, B.: MAGIX: Model Agnostic Globally Interpretable Explanations, *arXiv:1706.07160*
16. Ribeiro, M.T., Singh, S., Guestrin, C.: “Why Should I Trust You?”: Explaining the Predictions of Any Classifier. In: *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. pp. 1135–1144 (Aug 2016), 1602.04938
17. Russell, S.J., Norvig, P.: *Artificial intelligence. A modern approach*. Prentice-Hall series in artificial intelligence, Pearson Education Inc., Upper Saddle River, NJ, 3rd edn. (2010)
18. Strack, B., DeShazo, J.P., Gennings, C., Olmo, J.L., Ventura, S., Cios, K.J., Clore, J.N.: Impact of HbA1c Measurement on Hospital Readmission Rates: Analysis of 70,000 Clinical Database Patient Records. *BioMed research international* (2014). <https://doi.org/10.1155/2014/781670>
19. Wang, T., Rudin, C., Doshi-Velez, F., Liu, Y., Klampfl, E., MacNeille, P.: A Bayesian framework for learning rule sets for interpretable classification. *The Journal of Machine Learning Research* **18**(1), 2357–2393 (2017)
20. Wu, M., Hughes, M.C., Parbhoo, S., Zazzi, M., Roth, V., Doshi-Velez, F.: Beyond Sparsity: Tree Regularization of Deep Models for Interpretability. In: *Neural Information Processing Systems (NIPS) Workshop on Transparent and Interpretable Machine Learning in Safety Critical Environments* (2017), *arXiv:1711.06178*
21. Xie, P., Póczos, B., Xing, E.P.: Near-Orthogonality Regularization in Kernel Methods. *Uncertainty in Artificial Intelligence* (Aug 2017)
22. Xie, P., Zhang, H., Xing, E.P.: Learning Less-Overlapping Representations, *arXiv:1711.09300*
23. Zilke, J.R., Loza Mencía E., Janssen Frederik: DeepRED – Rule Extraction from Deep Neural Networks. In: *Calders, T., Ceci, M., Malerba, D. (eds.) Discovery Science*, pp. 457–473. *Lecture Notes in Computer Science* (2016)