Attention-like feature explanation for tabular data

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Abstract

A new method for local and global explanation of the machine learning black-box model predictions by tabular data is proposed. It is implemented as a system called AFEX (Attention-like Feature EXplanation) and consisting of two main parts. The first part is a set of the one-feature neural subnetworks which aim to get a specific representation for every feature in the form of a basis of shape functions. The subnetworks use shortcut connections with trainable parameters to improve the network performance. The second part of AFEX produces shape functions of features as the weighted sum of the basis shape functions where weights are computed by using an attention-like mechanism. AFEX identifies pairwise interactions between features based on pairwise multiplications of shape functions corresponding to different features. A modification of AFEX with incorporating an additional surrogate model which approximates the black-box model is proposed. AFEX is trained end-to-end on a whole dataset only once such that it does not require to train neural networks again in the explanation stage. Numerical experiments with synthetic and real data illustrate AFEX.

Keywords: machine learning, explainable AI, attention mechanism, pairwise interaction, neural network, tabular data

1 Introduction

An unprecedented growth of contribution of machine learning methods and models into solving various significant applied problems leads to requirements to explain the corresponding model predictions because most powerful machine learning models are very complex, for example, deep neural networks, their functioning is unclear due to the black-box nature of the models. The explanation problem is especially important in such applications as medicine, safety maintenance, finance, etc. A machine learning model user has to understand why the model predicts a certain decision, for example, a certain disease of a patient. This understanding may help to improve the user-model interaction and to justify the actions following the obtained prediction, for example, to choose the best treatment in accordance with the stated diagnosis [1]. The importance of explaining predictions provided by black-box models impelled to develop the corresponding explanation methods and models [2, 3, 4, 5, 6, 7, 8, 9, 10].

Depending on the instance set to be explained, there are local and global methods, which explain the black-box model predictions locally around a test instance and around a set of instance, for example, around the whole dataset, respectively. We focus on both the groups of interpretation methods, including local as well as global interpretations. Among the local explanation methods, the well-known method is LIME (Local Interpretable Model-Agnostic Explanation) [11], which belongs to methods based on constructing a surrogate model approximating the black-box model at a point. The surrogate model in LIME is the linear regression whose coefficients can be interpreted as the feature importance measures.

Another set of the explanation methods is based on applying Generalized Additive Models (GAMs) [12]. GAMs in the framework of explanation methods can be regarded as surrogate models which are represented as a sum of influence functions of features, i.e. the GAM outcome is a linear combination of
some functions of features. Several explanation models based on GAMs have been proposed, including the well-known Explainable Boosting Machine (EBM) [14], the Neural Additive Model (NAM) [15], GAMI-Net [16], the Adaptive Explainable Neural Networks [17]. The main peculiarity of the aforementioned surrogate models is that the influence or shape functions from GAM are obtained by training neural networks (in NAM or GAMI-Net) or by training the functions iteratively (EBM). There exist many other explanation models, for example, the SHapley Additive exPlanations (SHAP) [18, 19] and its various modifications. However, we draw attention mainly on the surrogate models which use GAMs as a basis for explanation because the proposed explanation method and its modification are also based on GAM to some extent. We propose a method which uses the attention-like approach. Therefore, we briefly consider the attention mechanism and its use in solving the explanation problems.

One of the important and efficient approaches for improving machine learning models is the attention mechanism which can be regarded as an extension of the Nadaraya-Watson kernel regression [20, 21]. It originally stems from a property of the human perception to selectively concentrate on an important part of information and to ignore other information [22]. Most applications of the attention mechanism focus on the computer vision area, including emotion detection, image-based analysis, visual question answering, etc., and the natural language processing (NLP), including text classification, translation, etc. Comprehensive surveys of attention mechanisms and their applications are provided by Chaudhari et al. [23], Niu et al. [22], Lin et al. [24]. Returning to explanation models, we can note that the idea to visualize attention weights jointly with an image instance directly leads to application of attention to solving the explanation or interpretation tasks. As a result, several studies discuss pros [25, 26, 27, 28, 29, 30] and cons [31, 32] of the attention application to problems of explanation. However, most results concerning with explanation by means of the attention mechanism are devoted to image-based analysis and NLP when inputs of a black-box model are represented as images or textual data, respectively. To the best of our knowledge, there are a few explanation methods (see, for example, [63]) using the attention mechanism for explaining tabular data.

Another important problem, which can be met in explanation, is a lack of efficient methods for identifying interactive effects or interactions between features when only combinations of two and larger features explain predictions of a black-box model. This problem has been partially solved in NAM and its modifications [15, 61, 16] where pairs of features can be fed to separate subnetworks and provide shape functions of two variables as outputs of these networks. The main obstacle for implementing NAM with pairs of features is that a huge number of subnetworks should be trained. Another way for considering interactions is to use EBM [14]. However, shape functions in EBM are gradient-boosted ensembles of trees such that each tree deals with a single feature or a pair of features. This also leads to a large number of trees for training. Moreover, EBM as an extension of the gradient boosting machine uses the greedy strategy which may lead to non-optimal solutions and incorrect results.

Taking into account the above, we propose a new attention-like explanation method which overcomes these difficulties and deals with tabular data. It uses many neural networks similar to NAM as its part and elements of a specific attention mechanism. That is why we use the term “attention-like” to characterize the proposed method. The method is implemented in the form of a system which is called AFEX (Attention-like EXplanation) and consists of several components, including, many neural networks (a set of one-feature neural subnetworks) for feature transformation, a specific scheme of the transformed features combining with the target values by means of the attention mechanism. The system parameters are trained by using the end-to-end gradient descend algorithm. In contrast to the original attention mechanism, we propose to combine not feature vectors with target values, but the data vectors corresponding to a single feature. In other words, a matrix of data (each instance is the corresponding columns) is transposed before applying the attention mechanism. The idea of this transposition is crucial and aims to assign weights to features which have a more strong connection with the corresponding target values. We propose the Feature attention instead of the standard Instance attention.

AFEX is trained on the whole set of points including points from the dataset and generated points around the dataset points. If the total explanation system shows convergence during training for all data,
then points from a small local area around an explanation point of interest from the area covering the training data can be processed without additional training of the system. This peculiarity defines the important property of universality. Moreover, it should be noted that some effects of features may not be detected on the local area especially, when there are global effects. In this case, it is better to detect effects on the whole set of data. The above does not mean that the method can be used only for the global explanation. It can be successfully applied to the local explanation. But the local explanation is obtained through the global one to some extent.

An important property of AFEX is that a basis of shape functions for every feature is constructed such that the final shape function of a feature is computed as the weighted sum of shape functions from the basis. Here the weights are obtained by using the attention mechanism. In other words, attention weights are used not for indicating the feature impact. They are for getting shape functions from subsets of basis shape functions.

Another idea behind AFEX or its modification for analyzing the pairwise interactions of features is based on pairwise multiplications of shape functions corresponding to different features. As a result, we do not construct many one-feature neural subnetworks plus a huge number of two-feature neural subnetworks. The pairwise multiplications of feature vectors are formed at the attention-like scheme.

In order to avoid the subnetwork overfitting, “a shortcut connection” with the trainable parameter is added to every subnetwork. Finally, we also consider a modification of AFEX, which is based on an additional surrogate model implemented as a simple neural network and trained jointly with other components of the system. This idea aims to cope with using a complex black-box model for getting predictions and to reduce the inference time of the whole system.

In summary, the following contributions are made in this paper:

1. We propose a new explanation method and its implementation AFEX for identifying important features as well as pairwise interactions between features, which, in contrast to GAMI-Net, is performed without quadratic growth in the number of neural subnetworks.

2. An important advantage of AFEX is that the whole system is trained end-to-end only once on an area of data around some central point such that the choice of a point for explanation in future does not require to train the neural subnetworks again, i.e., the feature contributions in the form of shape functions are obtained without additional training.

3. We propose to compute weighted sums of shape functions for every feature by using the attention-like mechanism. It is shown by numerical examples that the best attention is the linear regression which weights are recomputed at each forward pass.

4. Shortcut connections with the trainable parameter is used to avoid overfitting of neural subnetworks due to linearization of the basis shape functions corresponding to unimportant features.

5. We propose a modification of AFEX by adding a surrogate model implemented as a simple neural network and trained jointly with other components of the system. The modification improves the explanation system performance.

6. AFEX is illustrated by means of numerical experiments with synthetic and real data.

The code of the proposed algorithm can be found in https://github.com/andruekonst/afex.

The paper is organized as follows. Related work is in Section 2. A brief introduction to the attention mechanism and to NAM is given in Section 3. AFEX without considering pairwise interactions of features is introduced in Section 4. Pairwise interactions of features are considered in Section 5. The modification of AFEX with the additional surrogate model is studied in Section 6. Numerical experiments with synthetic data and real data are given in Section 7. Concluding remarks can be found in Section 8.
2 Related work

Local and global explanation methods. The need to explain black-box models led to development of many interesting explanation methods. One of the important methods is LIME [11]. Several modifications of LIME have been proposed due to its simplicity and clarity, for example, ALIME [33], LIME-Aleph [34], SurvLIME [35], LIME for tabular data [36], GraphLIME [37], etc. LIME and its modifications use the perturbation techniques [38, 39] which are based on generating many points around an explained instance and measuring how predictions are changed when features are altered [40]. The second important method, which motivated to develop many modifications, is SHAP [19]. It is based on a game-theoretic approach using Shapley values [18]. Several modifications and extensions of SHAP have been also proposed, for example, FastSHAP [41], Neighbourhood SHAP [42], SHAFF [43], X-SHAP [44], ShapNets [45], etc.

It should be noted that LIME and SHAP are only two approaches among many interesting methods which are successfully used in many applications. We do not consider many methods of counterfactual explanations [46], visual explanations [47] and other various methods which have been proposed to solve the problem of the machine learning model prediction explanation because LIME and SHAP can be regarded as a basis for developing several methods using GAMs for explanation. Comprehensive reviews providing details and peculiarities of most explanation methods can be found in survey papers [48, 49, 50, 51, 4, 52, 53, 54].

GAMs and NAMs in explanation problems. Due to flexibility and generality of GAM, this model has been successfully used for developing new local and global explanation models. In particular, explanation models based on the gradient boosting machines [55] to produce GAMs were proposed by [56, 57, 58]. Gradient boosting machines and GAMs were also used to construct the EBM [59, 14]. A differentially private version of EBMs called DP-EBM was proposed by Nori et al. [60].

A linear combination of neural networks implementing shape functions in GAM is a basis for NAMs [15] which sufficiently extend the available explanation methods and, in fact, open a door for constructing a new class of methods. Similar approaches using neural networks to construct GAMs and to perform shape functions are the basis of methods called GAMI-Net [16] and AxNNs [17]. An architecture called the regression network which can be also regarded as a modification of NAM is proposed by O’Neill et al. [61].

A method of applying GAM to recommendation system and taking into account feature interactions was proposed by Guo et al. [62] and is called GAMMLI. The neural GAM called NODE-GAM and neural GA^2M (NODE-GA^2M) models were proposed by Chang et al. [63] as an extension of NAM to deal with large datasets and to capture abrupt changes which cannot be detected by NAM. The models are based on using the neural oblivious decision trees [64]. A question of using a sparse GAM representation is studied in [59]. Application of NAM and the sparse GAM to solving the survival analysis problem under censored training data was also considered in [65].

3 Preliminary

3.1 Basics of the attention mechanism

It is pointed out in [23, 66] that the original idea of attention can be understood from the statistics point of view applying the Naradaya-Watson kernel regression model [20, 21]. Given n training instances

\[ S = \{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\} \]

in which \( x_i = (x_{i1}, ..., x_{id}) \in \mathbb{R}^d \) represents a feature vector involving d features and \( y_i \in \mathbb{R} \) represents the regression outputs, the task of regression is to construct a regressor \( f: \mathbb{R}^d \rightarrow \mathbb{R} \) which can predict the output value \( y \) of a new observation \( x \), using available training data \( S \). The similar task can be formulated for the classification problem.

The original idea behind the attention mechanism is to replace the simple average of outputs \( y^* = n^{-1} \sum_{i=1}^{n} y_i \) for estimating the regression output \( y \) corresponding to a new input feature vector \( x \) with the
weighted average in the form of the Naradaya-Watson regression model [20, 21]:

\[ y^* = \sum_{i=1}^{n} \alpha(x, x_i) y_i, \]  

(1)

where weight \( \alpha(x, x_i) \) conforms with relevance of the \( i \)-th training instance to the vector \( x \).

In other words, according to the Naradaya-Watson regression model, to estimate the output \( y \) of an input variable \( x \), training outputs \( y_i \) given from a dataset weigh in agreement with the corresponding input \( x_i \) locations relative to the input variable \( x \). The closer an input \( x_i \) to the given variable \( x \), the greater the weight assigned to the output corresponding to \( x_i \).

One of the original forms of weights is defined by a kernel \( K \) (the Nadaraya-Watson kernel regression [20, 21]), which can be regarded as a scoring function estimating how vector \( x_i \) is close to vector \( x \). The weight is written as follows [66]:

\[ \alpha(x, x_i) = \frac{K(x, x_i)}{\sum_{j=1}^{n} K(x, x_j)}. \]  

(2)

The above expression is an example of weights in nonparametric attention [66]. In terms of the attention mechanism [67], vector \( x \), vectors \( x_i \), and outputs \( y_i \) are called as the query, keys and values, respectively. Weight \( \alpha(x, x_i) \) is called as the attention weight. Therefore, the standard attention applications are often represented in terms of queries, keys and values, and the attention weights are expressed through these terms.

Generally, weights \( \alpha(x, x_i) \) can be extended by incorporating learnable parameters. For example, if we denote \( q = W_q x \) and \( k_i = W_k x_i \) referred to as the query and key embeddings, respectively, then the attention weight can be represented as:

\[ \alpha(x, x_i) = \text{softmax} \left( q^T k_i \right) = \frac{\exp \left( q^T k_i \right)}{\sum_{j=1}^{n} \exp \left( q^T k_j \right)}, \]  

(3)

where \( W_q \) and \( W_k \) are parameters which are learned, for example, by incorporating an additional feed forward neural network within the system architecture.

Several attention weights defining the attention mechanisms have been proposed for different applications. They can be divided into the additive attention [67] and multiplicative or dot-product attention [68, 69]. As pointed out by [22], the attention mechanisms can be also classified as general attention, concat attention, and a location-based attention mechanisms [68]. In particular, the general attention uses learnable parameters for keys and queries as it is illustrated in (parameters \( W_q \) and \( W_k \)). The concat attention uses the concatenation of keys and queries. In the location-based attention, the scoring function depends only on queries and does not depend on keys. A list of common attention types can be found in [22].

3.2 Neural additive model

AFEX has some elements which are similar to NAM [15]. Therefore, this approach is briefly described. NAM can be represented as a neural network consisting of many subnetworks (one-feature subnetwork) such that a single feature is fed to each subnetwork. The number of subnetworks is equal to the number of features in data. The \( i \)-th subnetwork implements a function \( g_i(x) \) which can be regarded as a univariate shape function in GAM. In other words, NAM implements GAM \( y(x) = g_1(x_1) + ... + g_m(x_m) \) under condition that functions \( g_i(x) \) are obtained by training the whole neural network with the loss function minimizing the expected difference between the whole network output \( y(x) \) and the target value \( y_j \) taken from training data. Subnetworks may have different structures, but they are jointly trained using backpropagation and can learn arbitrarily complex shape functions.

Details of the whole neural network training and testing are considered in [15].
NAM is a very efficient and rather universal method, and ideas behind NAM lead to new modifications and applications of the explanation method. In particular, a modification called SurvNAM dealing with censored data in the framework of survival analysis has been proposed in [65].

To implement the proposed attention-like explanation method, we do not use separately NAM. The idea of NAM to get functions $g_i(x_i)$ of single features is used to transform initial feature vectors. In AFEX, we use subnetworks, transforming features $x_i$, as elements of the whole system, i.e., we train the subnetworks jointly with other elements of the explanation system.

## 4 Description of AFEX

The main idea behind AFEX is to train a universal transparent explanation system that allows us to produce local and global explanations for any points of data by using information about the input features as well as about values of the target variable. Values of the target variable are used only for weighing the shape functions that depend on the input features.

Let us denote the vector of target values consisting of all outputs defined in a dataset $S$ as $y = (y_1, ..., y_n)$. An architecture of the proposed explanation system is shown in Fig. 1. Here $X$ is the matrix $d \times n$ of input features such that every column of the matrix contains values of one feature for all instances. Every row contains features of a single instance. For every feature, we train $k$ different one-feature neural subnetworks which compute $k$ different shape functions or shape vectors $g^j_i$, $j = 1, ..., k$, of the same feature $x_i$. Every shape function is a vector of size $n$, i.e., $g^j_i = (g^j_{i,1}, ..., g^j_{i,n})$, where $g^j_{i,t}$ is the value of the shape function for feature $x_i$ of the $t$-th instance produced by the $j$-th neural subnetwork. It should be noted that the subnetworks can be identical, but they do not share parameters. By means of $k$ subnetworks for a single feature, we get $k$ different feature representations or $k$ different shape functions. The total set of subnetworks is $k \cdot d$. Here $k$ can be regarded as a tuning parameter. Every $k$ shape function can also be viewed as a basis of functions such that every function in the shape function space can be represented as a linear combination of these basis functions with weights which will be considered below.

The result of the first part of the explanation system is $k \cdot d$ vectors of data corresponding to $d$ features, or $k \cdot d \cdot n$ values of shape functions, or matrix $F$ of the size $n \times (k \cdot d)$, where each column corresponds to the shape function $g^j_i$. Matrix $F$ is obtained by concatenating of $k \cdot d$ columns.

One of the important ideas behind AFEX is to find attention weights of all shape functions $g^j_i$ which establish the relationship between the shape function values and the target values $y$, i.e., between $g^j_{i,t}$ and $y_t$, $t = 1, ..., n$. In fact, subsets of the weights can be regarded as the basis function weights. If the weights were computed, we would find weighted sums of shape functions which show the feature behavior and their importance. So, the next step is to compute weights of the matrix $F$ columns.

Weights can be computed by different ways:

- By means of attention which is based on the dot-product with the softmax operation $\text{softmax}(y^T \cdot g^j_i)$ without a weighted matrix.
- By means of the correlation coefficient.
- By means of the linear regression.

All these approaches can be viewed as special forms of the attention mechanism. It is interesting to point out that the attention is applying to features but not to instances, i.e., we use the **Feature Attention** instead of the **Instance Attention**.

Suppose that we have computed the weights of the matrix $F$ columns. The next step aims to get the prediction $f(x_i)$ which is an approximation of $y_i$ for all $i = 1, ..., n$. It is performed by multiplying columns of matrix $F$ by the obtained weights $w_{ij}$ and then summing up results of the products.
The error backpropagation is used to train the whole explanation system. The loss function, for example, mean squared error (MSE), is defined as a distance between the predicted values (predictions of the explanation model) $f(x_i)$ and the target variable $y_i$. A batch is generated around a randomly selected point at each iteration of training, and the predicted values of the target variable are calculated using AFEX. Since the attention or linear regression weights are calculated in the differentiable way, the AFEX training is similar to the neural network training. As a result, if the training process converges, then, for any point of the training set, the weighted set of one-variable functions will provide a desirable approximation of the explained black-box model.

The next question is how to implement $k \cdot d$ neural subnetworks with one input feature. On the one hand, they should be large enough to approximate the function of the black-box model. On the other hand, they should not lead to overfitting. It is also important that each basic neural subnetwork should not have a negative effect on the training process of other subnetworks at initial stages of training. This implies that the initialization function has to be as simple as possible, for example, the linear one. The simplest way is to pre-train each neural subnetwork so that it approximates a linear function, but further training of the neural network may be difficult in this case.

Therefore, an alternative idea is proposed. According to the idea, a “shortcut connection” is added to every subnetwork as shown in Fig. 2. In contrast to the original shortcut connection used in the well-known ResNet [70], we replace the subnetwork with the linear combination of the linear function $x_i$ and the subnetwork output $h_{ij}^t(x_i)$ with the combination parameter $\alpha_{ij}$ such that the parameter $\alpha_{ij}$ is trainable. Its initial value is proposed to take as 0.9 to minimize the neural subnetwork impact, which is 0.1, and to maximize the linear function impact. This structure with the shortcut connection provides the shape function $g_{ij}^t = (1 - \alpha_{ij})h_{ij}^t + \alpha_{ij}x_{ij}$ for every instance with index $t = 1, ..., n$. During training, the combination parameter $\alpha_{ij}$ may be changed, and the model may implement an arbitrary complex function. If there exists some prior knowledge about the function implemented by each subnetwork, then a regularization can be used to realize functions which are close to the linear function.

It is important to note that parameters of AFEX in Fig. 1 including parameters of $k \cdot d$ neural...
subnetworks, weights of shape functions, linear combination parameters $\alpha_{ij}$, are jointly trained for the whole system by using the end-to-end learning process.

4.1 Attention-like differentiable regression

Let us consider an important part of AFEX which aims to compute weights of the matrix $F$ columns.

We propose to use a specific attention-like differentiable regression for computing the weights. Let us discuss other attention mechanisms which could be used in the proposed model, but are not used due to the following reasons. We write the scoring functions “score” estimating how vector $y$ is close to vector $g^j_i$ and used in the attention operations in terms of our task.

- The general attention [68]: $\text{score}(y, g^j_i) = y^T W_a g^j_i$. If matrix $W_a$ of the attention parameters is trainable, then a change of an order of instances in a batch leads to change of weights which become incorrect.
- The additive attention [67]: $\text{score}(y, g^j_i) = \tanh\left(W_a[y, g^j_i]\right)$. Similarly to the general attention, results may be incorrect if an order of points changes.
- The dot-product attention [68, 69]: $\text{score}(y, g^j_i) = y^T g^j_i$. Larger weights will be assigned to those features (columns of $F$) that have larger norms.
- The content-based attention [71]: $\text{score}(y, g^j_i) = y^T g^j_i/\|y\|\|g^j_i\|$. Weights depend on bias $b$, that is, adding a bias to the vector $\tilde{y}_j = y_j + b$ will change the weights. In AFEX, the training process is carried out on different local parts of the data domain, in which biases of the target variable are different.
- A procedure similar to the content-based attention with preliminary transformation of input vectors, where the average vector $\bar{y}^T$ (or $\bar{g}^j_i$) calculated over elements of each vector is subtracted from each vector $y^T$ (or $g^j_i$):

\[
\text{score}(y, g^j_i) = \frac{(y^T - \bar{y}^T) \left( g^j_i - \bar{g}^j_i \right)}{\|y^T - \bar{y}^T\| \|g^j_i - \bar{g}^j_i\|} \quad (4)
\]

This is the Pearson linear correlation coefficient. If there are correlated features, then their importance in significantly increases while the importance of other features may be significantly decreased.

In order to implement the attention-like regression for computing weights, we solve the following optimization problem

\[
w_{opt} = \left( \arg \min_w \|Fw - y\|^2 \right)^T, \quad (5)
\]
where matrix $F$ is non-square (the number of rows $n$ larger than the number of columns $k \cdot d$, i.e., $n > k \cdot d$); $w \in \mathbb{R}^{k \cdot d}$ is the vector of weights of the matrix $F$ columns; $w_{opt}$ is the vector of optimal weights by given $F$ and $y$.

One of the solution algorithms is the following:

1. Rank $r$ of matrix $F$ is determined.

2. If the rank is equal to the number of columns, then the QR decomposition is computed, for example, by using the PyTorch library which supports gradients computation through the block.

3. Otherwise, the problem is replaced with the problem

$$
\min_w \|(F^T F + \lambda I) w - F^T y\|^2,
$$

which is solved by means of the QR decomposition (we use in numerical experiments $\lambda = 0.1$).

Another question is how to compute weights in “Column weighting” (see Fig. 1) in case of the linear regression. To take into account the bias which differs for each new explanation area, matrix $\tilde{F} = (F; I)$ is constructed by adding a unit column to matrix $F$. Further, optimal weights $w_{opt} = \arg \min_w \|Fw - y\|^2$ are assigned to columns corresponding to features $\tilde{F}_{(i)} = g_i$ with the last weight corresponding to the bias.

If we replace the calculation of weights in the attention mechanism using the softmax score with the calculation of linear regression coefficients, then it turns out that finding the weights $w$ by the above method followed by weighting the input vectors represents the attention-like linear regression. If the weight vector $w$ in the original attention mechanism as the Naradaya-Watson regression model \cite{20, 21} ($y = \sum_i w_i g_i$) is defined as $w = \text{softmax}(\text{score}(y, g_i))$, then the attention-like linear regression is defined in a similar way, except the weights are determined by solving the problem (5).

To illustrate advantages of the attention-like linear regression, we perform the following experiment. Typical dependencies of the MSE as a function of the number of epochs for different methods of the weight computation are depicted in Fig. 3. We compare the following variants depicted in Fig. 3 when the black-box model is the function $x_1^2 + 0.5x_2$:

- Linear regression: the proposed approach, see (5).
- Correlation: see (4).
- Correlation+Softmax: see (4) and (3).
- Cosine: see the content-based attention \cite{71}.

It can be seen from Fig. 3 that the best convergence is observed for the linear regression. Similar relationships between different methods take place for other black-box model functions.

We have to point out that the linear regression is solved for every batch of data during training the whole system. In other words, trainable parameters of the system (weights of neural subnetworks) are modified after propagation a single batch of data, and new values of vectors $g_{1,(t)}, \ldots, g_{d,(t)}$ are computed, and they form matrix $F^{(t)}$, where $t$ denotes the training iteration number. New weights $w^{(t)}$ are calculated by solving the optimization problem (5) under condition that the matrix $F^{(t)}$ is computed at this iteration of the system training. As a results, $M$ iterations of the system training require to solve the problem (5) $M$ times. The training process is schematically depicted in Fig. 4 where the $t$-th iteration of the training is shown. One of the possible loss functions is

$$
\text{Loss}(F, w, y) = \|Fw - y\|^2.
$$

(7)
Figure 3: Comparison of different approaches to the column weighting

Figure 4: An enlarged scheme of the system training process
4.2 Testing (local explanation)

The testing process is schematically depicted in Fig. 5. $N$ points $x_1, ..., x_N$ are generated around an explained point. Predictions $y_1, ..., y_N$ are produced by the black-box model for all generated points. Matrix $F^*$ consisting of $N$ rows and $k \cdot d$ columns is generated by using the trained neural subnetworks. Matrix $F^*$ and vector $y = (y_1, ..., y_N)$ of predictions are used to solve the optimization problem (5) and to get vector $w_{opt}$ of weights of size $k \cdot d$. By multiplying every column of matrix $F^*$ by the corresponding weight from $w_{opt}$, we obtain $d$ vectors of feature contributions of size $N$ which, in turn, produce the shape functions that show whether the features are important or not.

5 An additional surrogate model

In order to improve AFEX, we propose to add a surrogate model which approximates the black-box model and is trained jointly with the main explanation model. The surrogate model is implemented as a neural network with some training parameters (weights of the network connections). An enlarged scheme of AFEX with the surrogate model is depicted in Fig. 6. The surrogate model is trained on the same dataset as the main explanation model. Its output is vector $z$ which can be regarded as an approximation of vector $y$. In contrast to the original explanation model, the linear regression block uses vector $z$ instead of $y$. As a result, the joint loss function takes into account both vectors $z$ and $y$. One of the possible loss functions is

$$\text{Loss} (F, w, y, z) = \|Fw - y\|^2 + \lambda \|y - z\|^2,$$

where $\lambda$ is the parameter which controls the strength of the second term.

It can be seen from the above loss function that neural networks producing matrix $F$ and the surrogate model are jointly trained and compensate each other. Another advantage of using the surrogate model is that we do not need to use the complex black-box model for getting predictions for all generated points around an explained point, the surrogate model copes with this task in a shorter time. Sometimes, there is a dataset, but the black-box model may be not available. In this case, we train the surrogate model and can investigate various points of the dataset.
6 Identifying pairwise interactions

One of the main reasons why AFEX is developed is to identify pairwise interactions among features. It turns out that the model can be simply modified for identifying the interactions. Interactions are said to exist when a change in the level of one factor has different effects on the response variable, depending on the value of the other factor [72]. In other words, the value of one feature modifies the effect of another feature and vice versa [73].

One of the most general approaches to identifying pairwise interactions between two features is the regression approach. According to this approach the interacted features are represented by multiplying the corresponding variables [73]. The idea of the feature multiplication can be realized by using the proposed model. In order to implement it, we propose to add a block which computes pairwise products of columns of matrix $F$. At that, only columns corresponding to different features are multiplied each other. Columns corresponding to the same features are not multiplied. The total number of obtained pairs is $k^2d(d-1)/2$, i.e., the matrix composed from the corresponding columns and denoted as $G$ consists of $k^2d(d-1)/2$ columns. In sum, the obtained matrix $G$ is concatenated with matrix $F$, and we get matrix $F^* = (F, G)$ consisting of $k^2d(d-1)/2 + kd$ columns and $n$ rows. This is depicted in Fig. 7. In fact, Fig. 7 illustrates a part of the total scheme shown in Fig. 1 such that matrix $F$ in Fig. 1 is replaced with matrix $F^*$ and the corresponding weights of columns are extended. Other parts of the total scheme remain without changes. The model is trained in the same way, however, the interpretation of results differs.

Each shape function depending on two features $x_i$ and $x_s$ is computed as a sum of shape functions of one feature with the corresponding weights $w_{ij} \cdot g_i^j$ plus the sum of shape functions of the second feature $w_{sl} \cdot g_s^l$ and the sum of products of shape functions with the corresponding weights $w_{i,s,t} \cdot g_i^j \cdot g_s^l$, i.e., $w_{ij} \cdot g_i^j + w_{sl} \cdot g_s^l + w_{i,s,t} \cdot g_i^j \cdot g_s^l$, where $t$ is the number of the pair $(j,l)$. It is important to note that the number of neural networks to take into account pairwise interactions does not increase in the proposed approach. This is a very important difference of the proposed approach from NAM [15] and its modifications, for example, regression networks [61]. Another advantage of the above approach in comparison with other approaches is that we get shape functions of pairs of features instead of some coefficients. A problem, which can be met in standard regression models taking into account the pairwise interaction, is how to interpret the coefficients of the corresponding products of variables. It is easy when features are binary. However, the interpretation in case of real-valued features can be incorrect. In contrast to these regression models, we obtain shape functions which can be interpreted in accordance with their...
7 Numerical experiments

7.1 Synthetic data

7.1.1 Combination of functions

To investigate AFEX and its peculiarities, in particular its property that the training can be carried out once, and explanations can be obtained for different local areas, the following numerical experiment is performed with synthetic data. Suppose that the black-box model is a function of two variables (features) of the form:

\[ I[x_1 \geq 0](x_0)^2 + I[x_1 < 0]x_0 \]

It is equal to the square of the first variable, \(x_0\), if the second variable, \(x_1\), is positive, otherwise, it is equal to the linear function of the first variable \(x_0\). Here \(I[A]\) is the indicator function taking value 1 if \(A\) is true. It is important to point out that this function cannot be approximated by GAM and NAM because these models do not deal with pairwise interactions.

The training process is performed with the batch size equal to 1000, instances are randomly generated from the uniform distribution with the expectation also generated randomly from the normal distribution with the standard deviation 1 at each iteration. After training, the obtained model is used to explain two different local areas around point \((0, 2)\) and point \((0, -2)\). These central points are taken to test two conditions \(x_1 \geq 0\) and \(x_1 < 0\). Points in the local areas are generated from the uniform distribution. Resulting shape functions for the first and the second areas (the first and the second rows of pictures) are shown in Fig. 8. It can be seen from the first row of pictures in Fig. 8 that the shape function for the first feature in the first case is close to a parabola, while in the second case, the shape function represents a linear function. The above implies that the single explanation model explains various areas of data.

To study the modification of the explanation method based on using the surrogate model, we realized the same experiment with this modification. The surrogate model is implemented as a neural network.
Figure 8: Shape functions explaining the model at two different local areas: the first and the second rows of pictures correspond to the areas around (0, 2) and (0, −2), respectively.

Consisting of 5 layers such that each layer has 10 units. The activation function is ReLU. The model has not been pre-trained. We again explain two different local areas around point (0, 2) and point (0, −2). Results are illustrated in Fig. 9. It can be seen from Fig. 9 that the proposed modification of AFEX with the surrogate model provides a more sensitive results.

7.1.2 Chessboard

The next numerical example demonstrates how AFEX copes with pairwise interactions of features. The black-box model is a function of five variables, which significantly depends on two (the first and the second) variables, and remaining variables do not affect the function values. We use the unimportant remaining variables because they may complicate the study of pairwise interactions due to possible overfitting the model. The function of the explained model is a “chessboard” with cells of size 2 × 2. Its formal writing is

\[ I \left[ (\sin \left( x_0 \cdot \frac{\pi}{2} \right) > 0) \neq (\sin \left( x_1 \cdot \frac{\pi}{2} \right) > 0) \right]. \] (10)

AFEX is trained by using batches of size 1000. Instances are randomly generated from a uniform distribution with a randomly selected center as in the previous numerical example, but the size of each local area is 0.5. Using AFEX, two different points are explained: the first one is close to the horizontal border between cells (the feature vector \( \left( \frac{1}{2}, 0, 0, 0, 0 \right) \)); and the second one is close to the diagonal junction of cells (the feature vector \( \left( 0, \frac{1}{2}, 0, 0, 0 \right) \)). The local area of generated instances is of size 1. Target values corresponding these two cases are shown in Fig. 10. Only two features are used for depicting target values because it is assumed that other features do not impact on target values.

Obtained shape functions of five features for the first local area around point \( \left( \frac{1}{4}, 0, 0, 0, 0 \right) \) are depicted in Fig. 11. The strongly marked step-wise shape function corresponding to the second feature, \( x_1 \), can be seen in Fig. 11. Indeed, if we look at the left picture in Fig. 10 then it is obvious that only change of the second feature leads to change of the chessboard cell. Moreover, this cell change is carried out at a point \( x_1 = 0 \) which corresponds to the shape function jump. It follows from Fig. 11 that shape functions of other features do not impact on the target values. This peculiarity also corresponds to Fig. 10 where it is clearly seen that changes of feature \( x_0 \) around \( x_0 = 0.5 \) does not change the cell. Other features do not impact on the target due to the assumption.
Figure 9: Shape functions explaining the model at two different local areas obtained by using the modification with surrogate model: the first and the second rows of pictures correspond to the areas around $(0, 2)$ and $(0, -2)$, respectively.

Figure 10: Areas around two points which are close to the horizontal border between cells (the left picture) and to the diagonal junction of cells (the right picture).
Let us consider the second point. For this point, there are dependences of target values on single features as well as on the pair of the first and second features. In order to see these pairwise interactions of features, we consider two-dimensional shape functions in the form of heatmaps illustrating how pairs of features impact on the target values. The heatmaps for some pairs of features, which show at least small changes, are depicted in Fig. 12. Numbers of features in each pair are indicated above the corresponding heatmap. It can be seen from Fig. 12 that the first heatmap corresponding to shape function of the pair of features $x_0$ and $x_1$ (pair $(0, 1)$) clearly illustrates that the proposed method copes with pairwise interactions of features (see also the right picture in Fig. 10). Other pairs of features are not important, and this fact is shown in the corresponding heatmaps whose colors are almost not changed.

### 7.1.3 Pairwise multiplication

We again consider a function of five variables, which is a simple product function $x_0 x_1$. Other variables $x_2, x_3, x_4$ do not impact on the target values. Let us take point $(1, 2, 1, 2, 1, 2)$ for explanation the corresponding prediction. When considering pairwise interactions, it makes sense to rely both on functions of pairs of features and on functions consisting of the sums of shape functions of each feature and the function of the pair. In this example, the black-box model is represented as the product of the first and second features. Functions depending on pairs of features are close to constant for all pairs of features, except for the pair $(0, 1)$. This fact can be seen from Fig. 13 where heatmaps of pairs of features are depicted similarly to Fig. 12. However, the dependence itself is not correctly represented because the largest values of function $x_0 x_1$ should be in the upper right corner and in the lower left corner. We have to add shape functions of the first and second features. In this case, we get a correct visualization of the dependence (see Fig. 14).

Adjusted shape functions are built as follows:

$$
w_{ij} \cdot g_i^j + w_{sl} \cdot g_s^l + w_{i,s,t} \cdot g_i^j \cdot g_s^l. \quad (11)$$

### 7.1.4 Vertical wedge

Let us consider a dataset which is generated by the function $I[2 \cdot |x_0| > |x_1|]$. This function looks like a vertical wedge (see Fig. 15). We again consider 5 features such that only two features are important. The example can be illustrated by two cases. In the first case, the black-box model provides predictions
Figure 12: Two-dimensional shape functions in the form of heatmaps illustrating how pairs of features impact on the target values in the second case of the chessboard example

Figure 13: Two-dimensional shape functions in the form of heatmaps illustrating how pairs of features impact on the target values for the example with function $x_0x_1$
in the form of integer values of classes (a classification problem). In the second case, the black-box model (the gradient boosting machine consisting of 100 trees with largest depth 3 and learning rate 0.1) provides probabilities of classes. Three points are taken for explanation: to the left (feature vector \((-1,2,0,0,0)\)) from the wedge, to the right (feature vector \((1,2,0,0,0)\)) from the wedge and in the center (feature vector \((0,1/2,0,0,0)\)). Fig. 16 depicts heatmaps illustrating how pairs of features impact on the target values for the first case of the “vertical wedge” example corresponding to three points \((-1,2,0,0,0), (1,2,0,0,0), (0,1/2,0,0,0)\), respectively. Only heatmaps for the pair of features \(x_0\) and \(x_1\) are shown because other pairs of features do not impact on predictions. It can be seen from Fig. 16 that it is possible to correctly approximate pairwise interactions of features for all three points. The same heatmaps for the second case, when probabilities of classes are used as predictions of the explained black-box model, are depicted in Fig. 17.

7.2 Real data

7.2.1 Boston Housing dataset

Let us consider the real data called the Boston Housing dataset. It can be obtained from the StatLib archive (http://lib.stat.cmu.edu/datasets/boston). The Boston Housing dataset contains 506 examples such that each example is characterized by 13 features. The explained black-box model is implemented as a neural network having 3 layers, every layer consists of 100 units with the ReLU activation function, and optimizer Adam is used for training on the Boston Housing dataset. The learning rate is \(10^{-3}\), the number of epochs is 1000. The proposed system is trained on generated local areas around randomly selected points from the whole dataset. \(N = 1000\) perturbed points are generated around the point of interest \(\mathbf{x}\) from the uniform distribution with bounds \(\mathbf{x}_{left}\) and \(\mathbf{x}_{right}\) defined as the 10%-interval of the feature range around point \(\mathbf{x}\) for explanation, and shape functions are constructed for the local explanation. Point \(\mathbf{x}\) for explanation is taken as the mean of two randomly selected instances from the Boston Housing dataset. We
Figure 15: Points of the dataset generated by the “vertical wedge” function

Figure 16: Two-dimensional shape functions in the form of heatmaps illustrating how pairs of features impact on the target values for the first case of the “vertical wedge” example corresponding to three points $(-1, 2, 0, 0, 0), (1, 2, 0, 0, 0), (0, 1/2, 0, 0, 0)$, respectively

Figure 17: Two-dimensional shape functions in the form of heatmaps illustrating how pairs of features impact on the target values for the second case of the “vertical wedge” example corresponding to three points $(-1, 2, 0, 0, 0), (1, 2, 0, 0, 0), (0, 1/2, 0, 0, 0)$, respectively
plot obtained individual shape functions for four important features “CRIM”, “LSTAT”, “DIS”, “B” in Fig 18. Similar results have been obtained in [56]. At that, one can see from the shape plots that contribution of feature “B” to the median value of the owner-occupied homes rises while contributions of other features are decreased.

7.2.2 Breast Cancer dataset

The next real dataset is the Breast Cancer Wisconsin (Diagnostic). It can be found in the well-known UCI Machine Learning Repository (https://archive.ics.uci.edu). The Breast Cancer dataset contains 569 examples such that each example is described by 30 features. The malignant and the benign are assigned by classes 0 and 1, respectively. We use the classification black-box model based on the SVM with the RBF kernel having parameter $\gamma = 1/m$ and the penalty parameter $C = 0.1$. We plot obtained individual shape functions for nine important features in Fig 19. Other features are not important because their shape functions do not change or their changes are very small in comparison with features whose shape functions are shown in Fig. 19. It is interesting to point out that features of the highest importance obtained in [56] for the same random point on the bases of the Breast Cancer dataset are “radius error”, “area error”, “worst area”, “worst symmetry”. All these features are included into the set of nine important features shown in Fig. 19.

7.2.3 California Housing dataset

Another numerical example is for comparing AFEX with NAM [15]. This is the California Housing dataset which can be found in the Kaggle (https://www.kaggle.com/camnugent/california-housing-prices). It contains 20640 observations with 9 features and aims to solve a regression problem to predict the median price of houses depending on several parameters. The explained black-box model is implemented as a gradient boosting machine with decision trees of depth 3. It is trained by using 100 iterations with the learning rate 0.1. A point for explanation is taken as a center of the dataset. It has the following values of features: “MedInc”=3.87; “HouseAge”=28.64; “AveRooms”=5.43; “AveBedrms”=1.1; “Population”=1425.5; “AveOccup”=3.1; “Latitude”=35.6; “Longitude”=−119.6. The global explanation as in [15] is studied, therefore, an area around the point is defined by lowest and largest values of all features. Shape functions of four important features “MedInc”, “Longitude”, “AveRooms”, “AveOccup” are depicted in Fig. 20. Other features cannot be viewed as important. The same results have been obtained by means of NAM.
However, the authors of [15] pointed out that only two features “MedInc” and “Longitude” should be regarded as important.

In order to study the pairwise feature interactions, we also construct heatmaps for pairs of features which can be viewed as important. They are depicted in Fig. 21. It is surprisingly seen from Fig. 21 that the pair of features “MedInc” and “Longitude” is important, but the pair “MedInc” and “AveOccup” is more important because small values of feature “AveOccup” lead to the crucial change of the feature contribution.

8 Conclusion

A new approach for solving the explanation problem of machine learning black-box model predictions has been proposed. System AFEX implementing the approach has several important advantages. First, AFEX identifies pairwise interactions between features in a simple way. Second, the system for a dataset is trained once and the local explanation of arbitrary points in the area of the dataset does not require to train again. Numerical experiments with synthetic and real data have demonstrated that AFEX correctly explain various difficult cases and datasets.

On the one hand, we have pointed out that shape functions may be a better way for representing results especially when pairwise interactions are studied. On the other hand, explanations are simpler for many users when they are represented by a single number measuring the feature importance. Therefore, development of approaches to represent shape functions, especially heatmaps, in a form of point-valued feature contributions is an interesting task for further research.

One of the ideas which has been proposed in AFEX is to multiply all pairs of columns corresponding to different features in order to realize the method for the pairwise interaction study. At the same time, the product of two vectors is one of the possible operations for taking into account the pairwise interactions. The flexibility of AFEX allows us to consider other operations different from the standard product. Study of these operations and investigation how they impact on the explanation results can be regarded as another
Figure 20: Shape functions of four important features learned on the California Housing dataset (the x-axis indicates values of each feature, the y-axis indicates the feature contribution to the median price of houses)

Figure 21: Two-dimensional shape functions in the form of heatmaps illustrating how pairs of features impact on the target values for California Housing dataset
Another problem of AFEX is that the number of neural subnetworks is equal to the number of features multiplied by the value of the basis shape functions $k$. Hence, high-dimensional datasets cannot be considered due to difficulties of training a huge amount of subnetworks. One of the ways to cope with this difficulty is to use a machine learning model different from neural network, for example, the gradient boosting machine. A justified selection of the best model for feature transformation is also a direction for further research and study.

We have applied only one differentiable model for computing weights, namely, the linear regression model. However, it is interesting to investigate whether AFEX can be improved by using another differentiable model, for example, SVM. This is another direction for research in future.

AFEX is developed for dealing with tabular data. Its modification for processing images, graph data, text information is also an interesting task for further research.

**Declaration of competing interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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