Explaining a prediction in some nonlinear models

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Abstract

In this article we will analyse how to compute the contribution of each input value to its aggregate output in some nonlinear models. Regression and classification applications, together with related algorithms for deep neural networks are presented. The proposed approach merges two methods currently present in the literature: integrated gradient and deep Taylor decomposition. Compared to DeepLIFT and Deep SHAP, it provides a natural choice of the reference point peculiar to the model at use.

1 Introduction and Motivation

Nonlinear models have been widely used especially for classification problems in many fields. Nevertheless, one of the main issues encountered by practitioners and academics is strictly related to the interpretation and explanation of the models’ output with respect to the input data. Indeed, focus on the issue dates back in the past also with respect to simple classifiers such as logit and probit. At the best of our knowledge, the first to approach output explanation with respect to some input data in non linear models using a stepwise Taylor decomposition were [Denk and Finkel (1992)]. They proposed a methodology to explain a change in a left hand side variable due to changes in right hand side variables. Further, they apply the method to presidential voting using the 1972-76 National Election Studies (NES) panel. Among the results in their paper, they conclude that, in logit models, a second order Taylor expansion is found to be enough for a \( \Delta x_j < \frac{0.5}{b_j} \); while, for higher differences among the right hand side variables, a stepwise method is advised by the authors. Successively, [Bazen and Joutard (2013)] provided theoretical foundation for using the Taylor decomposition to extend the Oaxaca method to nonlinear functions.

Nowadays, with a growing interest in machine learning tools from many fields, decision makers have sometime shown reluctance in those models because perceived as black boxes. Indeed, in disciplines such as economics, finance and healthcare, explaining predictions is as important as having a well performing model, see: [Tsang et al. (2017); Goodman and Flaxman (2017); Caruana et al. (2015)]. More in general, a graphical representation of model’s choices can help debugging it. Therefore, many scientists have dedicated their research focuses on trying to shed lights on decisions made by those models. A recent survey of the literature is provided by [Guidotti et al. (2018)]. Overall, methods present in the literature to explain models’ decisions could be distinguished in approaches involving auxiliary models fitting, and other solving the problem directly. Usually, the former provide less accuracy but more flexibility and therefore sometimes referred as agnostic, while, the latter more accuracy but at the cost of being applicable only to certain class of models.

1 Here for interpretation and explanation we mean the mapping of abstract concepts to the human world, and their graphical representation to explain a decision made by the model [Montavon et al. (2018)]

2 Formally, they drop crossproduct terms from the second order expansion.

3 Being not tied to a particular type of black box. Among the agnostic methods, the LIME technique from [Ribeiro et al. (2016)] is perhaps the most popular.

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In this work, we will present a method that is applicable only to a given class of models, but on the other side has maximal accuracy. Indeed, it is the researcher to define the approximation error. Moreover, the method is suitable both for classification and regression.

The algorithm proposed in this article merges two works: the integrated gradient (IG) of Sundararajan et al. (2017) and the deep Taylor decomposition (DTD) of Montavon et al. (2017). Regarding the DTD, it can be considered as an evolution of the layer-wise relevance propagation, technique first adopted in the pixel-wise decomposition method of Bach et al. (2015). The DTD consists in applying a Taylor decomposition in each neuron of the neural network, this allows a back propagation of the output towards its inputs.

A drawback of this methodology stands in the fact that the link function is not always well approximated by a one step first order Taylor decomposition, as shown for logit models in Denk and Finkel (1992).

On the other side, the IG approach could be interpreted as a generalization of the method proposed by Denk and Finkel (1992). It consists in carrying out a stepwise first order Taylor expansion of the neural network, where the initial root vector (so called baseline) could be found by imposing that the total output evaluated at this point is equal to zero.

As will be clearer in what follows, finding this baseline with respect to the full model is not always straightforward (especially when a theoretical baseline is not available). Nevertheless, it is trivial when the model is monotonic in each of its inputs. More so, there are cases where the output of the model is not in the set [0, 1], but for examples in all $\mathbb{R}^4$.

Two recent methods DeepLIFT of Shrikumar et al. (2017) and the Deep SHAP approach of Lundberg and Lee (2017), the former being a fast approximation of the latter, suffer the same problem related to the identification of the reference point.

Indeed, Deep SHAP suggests to use the expected values of the right hand side variables as reference vector; while, DeepLIFT proposes multiple references or user defined ones. Those issues have motivated our work, and the proposal of a novel algorithm.

The rest of the article is organized as follows. In section 2, we present theoretical support for our method, together with the algorithms that implement it; a comparison with related works will be done in this section as well. Section 3 is dedicated to empirical applications, both to a regression problem and to a classification one. Finally, section 4 concludes.

### 2 Explaining a prediction

When presenting the algorithms, we will be dealing with already estimated models. Therefore, we are not concerned with estimation. On the other side, we will be analysing explanation of a given conditional output with respect to its conditioning inputs, and given the optimal parametrization.

With this in mind, the attention is on decomposing a prediction and not on "what if" scenarios, which require modelling the dependences among right hand sides explicitly.

Additionally, and without loss of generality, inputs are assumed to be scaled to have zero mean and 1 standard deviation.

#### 2.1 Simple input-output models

In this section we propose a variation of the approach used by Denk and Finkel (1992) for logit models. The following Claim can be considered a formalization and generalization of it.

**Claim 1** Given a model of the form $y_t = G(y^*_t) = G(\beta^* x_t)$, with $G(.)$ being differentiable and monotonic in each of its inputs and with image in $[a, b]$, $\beta \in \mathbb{R}^K$ without loss of generality, and $x_t \in X$ bounded subset of $\mathbb{R}^K$, and $y^*_t \in Y$ bounded subset of $\mathbb{R}$, then approximate contribution of input $x_{t,k}$ is:

$$
\rho_{t,k} = \sum_{y^* = \beta^* x_0} g(y^*) \ast \beta_k \ast \Delta x_k + \frac{\beta_k}{\sum_{i=1}^{K} \beta_i} \ast a
$$

(1) Where $x_0$ is the starting root point, i.e., $x_{i,0} = c <= \text{min}(X) \forall i = 1, \ldots, K$ and $G(\beta^* x_0) = a$.

### Classification versus regression.
Using the definition of integral, that of derivative and by applying Taylor decomposition, we get:

\[ G(y_t) = \int_{-\infty}^{y_t} g(y) dy + G(-\infty) = \lim_{\Delta y \to 0} \sum_{t=0}^{y_t} g(y) \Delta y + a = \]

\[ \sum_{t=0}^{y_t} \lim_{\Delta y \to 0} G(y + \Delta y) - G(y) + a = \sum_{t=0}^{y_t} \lim_{\Delta y \to 0} \sum_{n=1}^{\infty} \frac{G^{(n)}(y)}{n!} \Delta y^n + a. \]

Where \( g(.) \) stands for the first derivative of \( G(.) \) with respect to its argument, and \( G^{(n)}(.) \) for the \( n \)-th derivative. It is worth noting that \( G(y) \) disappears, only its derivatives and the starting point (or baseline) are left.

If we want the contribution of each of the terms to be additive and to sum up to the total output (Montavon et al. [2017] refer to an heatmap with this property as a conservative one), then we need to truncate the Taylor expansion to the first order.

The numerical integration is required to avoid loosing accuracy when truncating the Taylor expansion. Clearly, the higher is the degree of non linearity of the function \( G(.) \), the bigger will be the gain in accuracy provided by the numerical integration.

Hence,

\[ G(y_t) \approx \sum_{t=0}^{y_t} g(\beta x) \ast (\beta' \Delta x) + a = \sum_{t=0}^{y_t} g(\beta x) \ast (\beta_1 \Delta x_1 + \ldots + \beta_K \Delta x_K) + a. \]

For a small enough \( \Delta x_k \) the approximation error gets negligible.

We should now define the starting point of the numerical integration, i.e.: the initial root point for the Taylor expansion.

Assuming \( G : X \to [a, b] \), for observation \( x \) the initial root point is found by solving the following constrained minimization problem (Montavon et al. [2017]; Szegedy et al. [2013]):

\[
\min_{\theta} || \theta - x ||^2 \quad \text{subject to } G(\theta) = a \quad \text{and} \quad \theta \in X \tag{2}
\]

This minimization problem is not necessary solvable. Nevertheless, when \( G(\theta) \) is monotonic in each of its inputs and \( |a| < \infty \) the problem is trivial and can be solved easily\(^6\).

Hence,

\[ G(y_t) \approx \sum_{t=0}^{y_t} g(\beta x) \ast (\beta_1 \Delta x_1 + \ldots + \beta_K \Delta x_K) + G(\beta \ast x_0). \]

It is left to redistribute the starting point \( a = G(\beta \ast x_0) \) with respect to each of the features\(^6\).

Given a small \( \epsilon > 0 \), we can explain the variation \( G(\beta \ast (x_0 + \epsilon)) - G(\beta \ast x_0) \) with respect to \( x_i \) \( \forall i = 1, \ldots, K \). Following the reasoning above, this is given by \( \beta_i g(\beta x_0) \ast \epsilon \).

Therefore, the fraction of \( a \) explained by variable \( x_i \) is: \( \frac{\beta_i}{\sum_{j=1}^{K} \beta_j} \ast a. \)

In case of singe layer classifier \( G : X \to [0, 1] \), the algorithm implements as follows.

**Algorithm 1** Steps to explain simple classifiers

1. Store the parameters from your model estimated on standardized \( X \)

2. (Searching Initial Root Point) Solve optimization problem in Equation (2) and get \( X_{\text{base}} \)

3. Define the number of grid points (you can make it proportional to the distance between the current \( X \) and \( X_{\text{base}} \))

4. Generate the matrix of observations such that for every \( x_i \) you have all the values from \( X_{\text{base}} \) to the current observation \( x_{i,1} \) with constant delta dependent on the number of grid points defined above and on the distance between the root point and the current observation

5. Apply formula in equation (1). Sum up all the contributions and check the difference with the prediction of your model. If it is too high, then increase the number of grid points

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\(^6\)One remark that must be made is that with multilayer models this problem could not have a solution due to constraints on the input space \( X \) coming from the previous layer. In practice, we found this issue only when setting high and unreasonable thresholds for the classification problem analysed in section 3.2.

\(^7\)We provide explanation also for the baseline for a matter of completeness; indeed, sometime the researcher could be not interested in this, as its focus could be on explaining the difference with respect to it. Nonetheless, this is useful for regression problems.
2.2 Deep neural networks

In this section we will apply the method to explain a prediction coming from a fully connected multilayer perceptron (MLP) with respect to its input data. To note that the algorithm proposed does not apply only to classification problems. Indeed, in the next section we will present an application to a regression problem.

While we provide examples for those networks, with relatively minimal adjustments to the algorithm, applications to more complex deep neural nets can be carried out.

In principle, any non linear model that can be decomposed into trivial functions (what this stands for will be clearer soon), and non-trivial functions satisfying assumptions made in Claim 1 can have its predictions decomposed as discussed in this article.

When the MLP under analysis satisfies the conditions to deliver a unique solution to the optimization problem in (2) or a theoretical grounded baseline for the right hand side variables is provided by the researcher, then one can apply the IG method of Sundararajan et al. (2017). Otherwise, the algorithm for the general case is presented here below.

Algorithm 2 Steps to explain deep neural networks: deep explanator (DE)

Let’s first define two sets of link functions. Being $\Theta$ the set of all the link functions and $\Omega \subset \Theta$ the one with trivial functions (i.e.: any link function whose derivatives are constant once the output of that link function is known; linear, ReLU and its generalizations are such cases being the impact constant or constant given the output), we can define the set of non-trivial link functions: $\Phi = \Theta \setminus \Omega$.

1. Store the parameters from your model estimated on standardized $X$
2. Starting from the first layer, loop over its neurons and compute the contribution of each input to the current output
3. When computing the contribution check if the function is in set $\Phi$; apply the stepwise Taylor expansion only in this case (Algorithm 1)
4. Do so for every layer
5. You will get $NH + 1$ matrices for each observation; where $NH$ is the number of hidden layers
6. Finally, multiply all these matrices and you will get the contribution of each input to the output
7. Sum over the contributions and check whether the approximation error is too high. If so, then increase the number of grid points

Additionally, and in case of a classification problem, one could have estimated an optimal threshold $a$ according to some method (as in Sarlin and von Schweinitz (2017) or Alessi and Detken (2011)), and therefore be interested in explaining the contribution toward model’s decision. This can be achieved by finding the root point $c$ (and its associated root vector) for the neurons in the last hidden layer that makes the link function of the output layer $G(\cdot)$ computed at this point equal to the desired threshold $a$. Then application of Algorithm 1 will deliver to the contribution of the neurons in this layer to the output. Back propagation of this procedure delivers to the final decomposition with respect to the input features.

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7One method to achieve this is by imposing constraints in the network structure as in Dugas et al. (2009).
8We apologize for possible confusion with the deep explanator of Deep LIFT, but at the time of the first draft of this paper we were unaware of other methodologies out of IG and DTD.
9In practice, the number of matrices between input and first hidden layers varies depending on when the search of the root point need to be applied and how many layers are in the structure. For example, in case of a classification problem with 2 hidden layers you will have $N_{HL2}$ matrices of size $N_{HL1} \times N_{IL}$, where $N_{i}$ is the number of neurons in layer $i$; this arises because of the different root vectors coming from solving different problems in (2), as the function $G(\cdot)$ is parametrize with different weights and biases. Therefore, and assuming the same number of neurons $n$ in each hidden layer, computational cost is of the order $n^{HL}$ where $HL$ is the number of hidden layers.
10All matrices but the one of the first layer need to be manipulated in order to isolate the neuron impact from its size (therefore, only the coefficient need to be taken).
3 Empirical applications

In this section we will apply Algorithm 2 to two problems: regression and classification. The purpose of this section is to show how an intuitive graphical representations can be carried out. Therefore, we will not focus on the models’ performances and their structures are defined solely for illustrative purposes.

3.1 Application to a regression problem

For the regression problem we consider the American Housing Survey dataset. This is the same dataset used in Mullainathan and Spiess (2017), and consists of 162 features with 51808 observations. We fit a DNN with 2 hidden layers. Namely, a linear link function connects the initial 162 inputs to the first hidden layer with 16 neurons, then those neurons are connected via a tanh link to the second hidden layer with 4 neurons, which are finally mapped to the total output via a linear aggregation.

Figure 1 shows a stacked bar chart for the decomposition of the aggregate output, together with predicted and actual standardized values for 20 observations. The 162 initial features are mapped to 6 groups according to the topic; while, the contribution of biases is cumulated.

3.2 Application to a classification problem

When it comes to classification, we use the Pima Indians Diabetes dataset from the National Institute of Diabetes and Digestive Kidney Diseases, as in Maniruzzaman et al. (2018). In the dataset there are a total of 8 features. We use again a DNN with 2 hidden layers. A linear function maps those 8 features to 6 neurons, then ReLU link reduces them to 4, ultimately a sigmoid makes the final aggregation.

Figure 2 provides decomposition on the first 20 observations of the test set (20% of the overall data).

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11Python codes to replicate figures are available upon request. We used the SciPy package to solve for optimization problems as in equation (2).
12Those 20 are taken as the first observations of the test set part, which accounts for 20% of the overall data.
13The dataset can be found at this GitHub link: https://raw.githubusercontent.com/jbrownlee/Datasets/master/pima-indians-diabetes.data.csv. Original donor is Vincent Sigillito.
14We cite only the most recent paper and refer to the bibliography in there for the interested reader.
Figure 2: Explanation of DNN predictions - classification using the Pima Indians Diabetes dataset. Red line is predicted probability minus reference point (right axis), while blue dots are actual values (right axis).

768 data points). Here we set a threshold for the decision rule. Therefore, values can be directly interpreted as contributions to the final classification decision. Observations on the red line are computed as predicted probabilities minus the threshold estimated with balanced preferences towards type one and two errors (as in [Alessi and Detken (2011)]). Hence, every time the red line is above 0 (right axis) the model classifies the observation as positive.

4 Conclusion

In this article, after briefly discussing current methods used to explain predictions in some non-linear models, we have proposed a new approach that merges two of the ones present in the literature. In particular, the deep explanator (DE) presented in Algorithm 2 has been motivated by the weaknesses found in current state of the art methodologies.

Namely, it facilitates the search of the baseline (initial root point) by exploiting the monotonicity of each of the link functions. More so, it maintains high accuracy, thanks to the numerical integration. As such, the method is suited for researchers that do not have in mind a specific baseline for the right hand side variables.

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