A point-wise linear model reveals reasons for 30-day readmission of heart failure patients

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Abstract
Heart failures in the United States cost an estimated 30.7 billion dollars annually and predictive analysis can decrease costs due to readmission of heart failure patients. Deep learning can predict readmissions but does not give reasons for its predictions. Ours is the first study on a deep-learning approach to explaining decisions behind readmission predictions. Additionally, it provides an automatic patient stratification to explain cohorts of readmitted patients. The new deep-learning model called a point-wise linear model is a meta-learning machine of linear models. It generates a logistic regression model to predict early readmission for each patient. The custom-made prediction models allow us to analyze feature importance. We evaluated the approach using a dataset that had 30-days readmission patients with heart failures. This study has been submitted in PLOS ONE. In advance, we would like to share the theoretical aspect of the point-wise linear model as a part of our study.

1 Introduction
Seven decades after the birth of the learning machine [1], we now have deep learning neural networks (NNs) that provide various predictive analyses of electronic medical records (EMR) [2–7]. Nonetheless, chronic diseases such as heart failure (HF) still need more compelling and innovative strategies to decrease treatment costs [8]. Notably, from 2013 to 2014 the annual HF cost including the indirect cost was an estimated $327.7 billion in the United States (US) [9]. HF treatment costs due to hospital admissions are the most expensive element of this bill [8], so predictive analytics is an area of promise for controlling rising hospitalization costs and improving the outcomes of HF patients.

Various studies have developed predictive models for unplanned hospital readmissions [10]. Ouwerkerk et al. compared prediction models (177 models in 55 papers) for mortality and/or HF hospitalization by using C-statistic values [11]. Notably, they found reported that predicting HF (C-statistic: 0.68 ± 0.001) was more complicated than predicting mortality (C-statistic: 0.71 ± 0.001). Recent studies are testing whether deep learning methods, which can take into account heterogeneous EMR data (e.g., diagnoses, medications, laboratory test results, and diagnosis notes) and nonlinear

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interactions between predictors of HF readmission perform better than other methods\cite{2,4,7}. Deep learning models are thought to predict early readmission from such data more accurately than conventional statistical models. Interestingly, the previous studies did not use deep learning models to examine which features are important in predicting early readmission. While accurate prediction models would incorporate sophisticated knowledge that could reveal reasons for the readmission of HF patients, as Turing once suggested, an important feature of a learning machine is that we will often know almost nothing about exactly what is going on inside it\cite{1}. As long as we use only the results of deep learning, we will not be able to gain knowledge that could be used for preventing readmissions.

Deep learning models are neural networks (NNs) with deep layers, each of which has several hidden neurons receiving input from combinations of the neurons in the previous layer. The pipelines between hidden neurons express complex interactions between the input features. Among the deep learning models that have been remarkably effective in the fields where the interactions of the input features should be taken into consideration are the convolutional neural networks (CNNs) used in image analysis\cite{12} and the recurrent neural networks (RNNs) used in language processing\cite{13}. Medical informatics should also be a field to which deep learning can contribute because human health depends on a lot of biological elements related to each other. As deep learning technology spreads into more and more applications, there is a growing need to explain the reasons for its predictions. In fact, to make deep learning models explainable, a lot of methods have been devised to measure the importance of individual features, i.e., how much each feature contributes to the output. These methods can be roughly classified into perturbation-based and saliency-based ones. Perturbation-based methods calculate the importance score on the basis of how the output behaves in relation to perturbed input\cite{14,16}. The problem with them is their high computational cost: these methods require a large number of perturbations to be generated around each sample’s input and make all the perturbed input for all the samples propagate through the whole network. In saliency-based methods, on the other hand, the importance score depends on the saliency of each feature evaluated by the gradient of output with respect to the input\cite{17,20}. Saliency-based methods are computationally inexpensive because this gradient can be calculated in a single backward pass.

In this paper we present a point-wise linear model, a new algorithm for constructing innately explainable deep learning models. In the usual deep learning models, the network computes new feature vectors whose linear combination adequately expresses the objective model. The network of the point-wise linear model, in contrast, derives a weight function for each original feature vector as a function of the original feature vectors. The weighted sum of the original feature vectors with these weight functions gives the objective model. Since the weight functions depend on the original feature vector, the model, unlike a simple linear model, involves the nonlinear interactions between the original features. Because the model is a simple weighted sum of the original feature vectors, the importance of each feature can be evaluated by its weight function, as in a linear model.

Our method has two novel properties. One is that the importance is computed in the same way as in a linear model, a traditional model with which medical informatics experts are very familiar. This property is highly advantageous in medical applications because one can use the know-how of medical-data analysis accumulated throughout its long history. LIME\cite{16}, a model that produces a linear model for each data point by sampling perturbed data points, also has this advantageous property but, like other perturbation-based methods, is exceptionally computationally expensive. In contrast, our method produces an explainable model and incurs no extra computational time to compute importance scores other than the time for training the time for training the model: this is the other novel property of our method. The saliency-based methods are also free from the computational-cost problems, but they do not have the familiarity of a model computing importance the way a linear model does. In Layerwise Relevance Propagation\cite{19} and DeepLIFT\cite{20}, for example, the importance score is derived from how much the output deviates when the input differs from some reference value. It is difficult to compare this score with the results of previous medical studies. In contrast, linear and piecewise linear models such as logistic regression, random forest, and gradient boosting can provide feature importances explaining what learning machines (or models) are doing. A deep learning model accurately predicting the readmission of HF patients might use unknown and nonstandard knowledge that could improve the treatment of HF. We have therefore devised a means of explaining the deep learning models in order to provide tailored feedback to physicians.

This preprint shared the part of the materials and methods sections dealing with explainable deep learning. Experiments will be published in PLOS ONE.
2 Point-wise linear models

In this section we summarize why usual deep learning models are not explainable and then propose the point-wise linear model, our explainable deep learning model. We assume in this paper that in any vector space the inner product is defined by the dot product. The notation $v(u)$ for arbitrary vectors $v$ and $u$ indicates that every element of $v$ is a function of the elements of $u$. Additionally, we use the Einstein summation convention and a Greek-character subscript index to indicate components of a vector.

2.1 Idea of point-wise linear models

Let $x^{(n)} \in \mathbb{R}^D$ ($n = 1, \ldots, N$) represent a feature vector with $N$ denoting the sample size and $\mathbb{R}$ indicating the real number set. Firstly, we defined a logistic regression model as follows:

$$y^{(n)} = \sigma(w^{(n)} \mu), \quad (1)$$

where $w \in \mathbb{R}^D$ is a weight vector for $x^{(n)}$, $\sigma$ is a sigmoid function, and $y \in \mathbb{R}^D \{0 \leq y^{(n)} \leq 1\}$ is a probability value such as readmission probability for a patient. For simplicity of notations in these subsections, bias parameters have been removed from Eq (1) and other equations with learning weights. Fig 1 (a) shows the network architecture of the logistic regression model. The weight vector $w$ is bound to the feature vector $x^{(n)}$. We can understand the importance of each feature variable by analyzing the magnitude of the element in $w$.

Next, we give a usual deep learning model as shown in Fig 1 (b). A new feature vector $\varphi^{(n)}(x^{(n)}) \in \mathbb{R}^{D'}$ is nonlinearly generated from the original feature vector $x^{(n)}$. (b) shows a fully connected neural network. $\varphi^{(n)}$ and $w'$ are an inner vector and learning parameters, respectively. (c) shows a point-wise linear model. The upper block in (c) is a meta-machine generating a learning parameter $\xi^{(n)}(x^{(n)})$ in Eq (5). The lower block in (c) is a logistic regression model for each feature vector $x^{(n)}$.

Figure 1: Comparison of network architectures. (a) shows a logistic regression model. $x^{(n)}$ and $y^{(n)}$ are a feature vector and a target value ($(n)$ is sample index), respectively. $w$ is a vector of learning parameters for $x^{(n)}$. (b) shows a fully connected neural network. $\varphi^{(n)}$ and $w'$ are an inner vector and learning parameters, respectively. (c) shows a point-wise linear model. The upper block in (c) is a meta-machine generating a learning parameter $\xi(x^{(n)})$ in Eq (5). The lower block in (c) is a logistic regression model for each feature vector $x^{(n)}$.

Next, we give a usual deep learning model as shown in Fig 1 (b). A new feature vector $\varphi(x^{(n)}) \in \mathbb{R}^{D'}$ is nonlinearly generated from the original feature vector $x^{(n)}$ through the following $L$-layer neural network:

$$\varphi(x^{(n)}) = \sum_{\alpha=1}^{D} a^{(n)} \cdot b^{(n)}$$

$A_{\alpha \beta}B_{\beta \gamma} \equiv \sum_{\beta=1}^{D} A_{\alpha \beta}B_{\beta \gamma}$ for arbitrary $D$-dimensional vectors $a$ and $b$. $A_{\alpha \beta}B_{\beta \gamma}$ for arbitrary $D$-dimensional tensors $A_{\alpha \beta}$ and $B_{\beta \gamma}$.
network (NN):

\[ \varphi(x^{(n)}) = f^{(L)}g^{(L)} \ldots f^{(l)}g^{(l)} \ldots f^{(2)}g^{(2)}f^{(1)}(x^{(n)}), \]

where \( f^{(l)} \) is an activation function such as sigmoid, tanh, or ReLU. The function \( g^{(l)} \) is expressed as

\[ g^{(l)}(x) = W^{(l)}x, \]

where \( W^{(l)} \in \mathbb{R}^{D_{l+1} \times D_l} \) \((D_{l+1} = D \text{ and } D^{(L+1)} = D')\) is a weight matrix. The pair of functions \( f^{(l)} \) and \( g^{(l)} \) is called “the \( l \)-th inner layer”. A deep-learning-based nonlinear classification function predicts probability \( y^{(n)} \) as follows:

\[ y^{(n)} = \sigma(w'_\mu \varphi(\mu)(x^{(n)})), \]

where \( w'_\mu \in \mathbb{R}' \) is a universal weight vector for \( \varphi \). The magnitude of each \( w'_\mu \) element represents the contribution of the corresponding element of \( \varphi \) to the prediction as shown in Fig 2(b). However, one cannot “explain” the machine’s prediction by \( w'_\mu \) because one cannot understand the meanings of the new feature vector \( \varphi \) with which the machine makes its predictions.

In order to make a deep NN explainable, we considered a meta-learning to generate a logistic regression model defined as

\[ y^{(n)} = \sigma(\xi(\mu)(x^{(n)})x^{(n)}), \]

where each element of \( \xi \in \mathbb{R}^D \) is a function of \( x^{(n)} \) that the NN determines. \( \xi \) behaves as the weight vector for the original feature vector \( x^{(n)} \). The magnitude of each element of \( \xi \) describes the importance of the corresponding feature variable. Unlike \( \varphi \), the original vector \( x^{(n)} \) is comprehensible, and hence the model defined by Eq (6) is “explainable.” Here we should notice that this weight vector is tailored to each sample because \( \xi \) depends on \( x^{(n)} \). We call Eq (5) a point-wise linear model over the sample index \( n \). The architecture of the point-wise linear model consists of two blocks as shown in Fig 1(c). The upper block is a meta-learning machine of logistic regression models. The lower block is the logistic regression model for the inference task. In the following subsections we introduce two techniques for constructing the point-wise linear models.

### 2.2 Straightforward model

As one simple way to construct the weight vector, we considered a matrix \( \tilde{W}_l \in \mathbb{R}^{D \times D'} \) that transforms the nonlinear feature vector \( \varphi \in \mathbb{R}' \) into a vector in the original feature space \( \mathbb{R}^D \):

\[ \eta_\mu(x^{(n)}) = \tilde{W}_\mu \varphi(x^{(n)}), \]

where \( \eta \in \mathbb{R}^D \). We can construct a point-wise function in a straightforward manner by defining \( \xi \) in Eq (5) as

\[ \xi(x^{(n)}) = \eta(x^{(n)}). \]

To train the meta-learning machine Eq (5) path through Eq (7), we minimized the negative log likelihood (NLL) loss of the output \( y^{(n)} \) for the target label \( t^{(n)} \) := \{0, 1\}:

\[ \min_{\eta, \xi} \sum_{n=1}^N t^{(n)} \log \left[ \sigma(\xi(\mu)(x^{(n)})x^{(n)})) \right] + (1 - t^{(n)}) \log \left[ 1 - \sigma(\xi(\mu)(x^{(n)})x^{(n)}) \right]. \]

To investigate the performance of the explainable point-wise linear model given by Eq (5) with (7), we trained a simple toy dataset (sklearn.datasets.make_circle) by using the straightforward model, the logistic regression model (Eq (1)), and a self-normalizing neural networks (SNNs) model as a state-of-the-art NN model. The circle in a circle is not a linearly separable problem, so as shown in Fig 2(b), the logistic regression model could not classify the two circles. The SNNs correctly classified the blue and orange dots as shown in Fig 2(c) (21). On the other hand, the point-wise linear model (Eq (5) with Eq (7)) tried to learn the labels of all samples as it generated a weight vector optimized for each sample, which led to overfitting in Fig 2(d). The next section describes another approach to generating a point-wise linear function, an approach that overcomes the overfitting problem.
Figure 2: Classification results for a simple toy dataset. (a) is a large circle (orange dots) that contains a smaller circle (blue dots) obtained by `sklearn.datasets.make_circle`. (b) and (c) are the boundaries classified by the logistic regression model and self-normalizing networks (SNNs) model, respectively. (d) and (e) are the boundaries classified by the point-wise linear model of the straightforward model Eq (7) and the reallocation-based model Eq (9), respectively. (f) is the boundary classified by the reallocated feature vectors $\rho$. (g) is the arctangent of the angle between the horizontal and vertical elements of the weight vector $\xi^{(n)}$. The weight vector smoothly changes for each data sample.

2.3 Reallocation technique

We propose an alternative point-wise linear model by using instead of Eq (7)

$$\xi^{(n)}(x^{(n)}) \equiv w \odot \eta(x^{(n)}),$$

where $\eta$ is defined in Eq (6), $w \in \mathcal{R}^D$ is a universal weight vector that is independent of $x^{(n)}$, $\odot$ is the Hadamard product. $\xi^{(n)}$ gives a weight vector for each sample $x^{(n)}$. As in Eq (5), we can analyze the magnitude of $\xi^{(n)}$ for each dimension in the original feature space with which the machine makes decisions. In contrast to the model defined by Eq (7), the model defined by Eq (9) accurately predicts the classification boundary, as shown in Fig 2(e). The weight vectors $\xi^{(n)}$ in Eq (9) smoothly change for each data sample (Fig 2(g)). The reallocation-based point-wise linear model thus enables generalization.

To clarify the mechanism of the alternative point-wise linear model, we reformulated Eq (5) with Eq (9) as follows:

$$y^{(n)} = \sigma \left( \left( w \odot \eta(x^{(n)}) \right)_{\mu} x^{(n)}_{\mu} \right)$$

$$= \sigma \left( w_{\mu} \left( \eta(x^{(n)}) \odot x^{(n)} \right)_{\mu} \right)$$

$$\equiv \sigma \left( w_{\mu} \rho_{\mu}(x^{(n)}) \right).$$

(10)

We call $\rho(x^{(n)}) \equiv \eta(x^{(n)}) \odot x^{(n)}$ a reallocated feature vector in $\mathcal{R}^d$. NNs have a versatile ability to map a linear feature space to a nonlinear feature space. By utilizing this ability, Eq (10) reallocates the feature vector $x^{(n)}$ into the new vector $\rho$ that is linearly separable by a single hyperplane drawn by $w$. Additionally, one can impose a limit on the reallocation by

$$\rho(x^{(n)}) = C \left( \eta(x^{(n)}) \odot x^{(n)} \right),$$

(11)

where $C$ is a clamp function that operates on each vector element as follows:

$$C(x) = \begin{cases} 
\min & \text{if } x < \min \\
\max & \text{if } \min \leq x \leq \max \\
x & \text{if } \max < x 
\end{cases}.$$
where \( \alpha \) is a mixing parameter with \( 0 \leq \alpha \leq 1 \).

### Table 1: Variations of the reallocation functions.

| Type | Transform function | Transform weight | Reallocation function |
|------|--------------------|-----------------|----------------------|
| I    | \( u^{(n)} = \eta(x^{(n)}) \) | \( W \in \mathbb{R}^{d \times d'} \) | \( \rho(x^{(n)}) = u^{(n)} \odot x^{(n)} \) |
| II   | \( u^{(n)} = \eta(x^{(n)}) \) | \( W \in \mathbb{R}^{d \times d'} \) | \( \rho(x^{(n)}) = u^{(n)} + x^{(n)} \) |
| III  | \( (u^{(n)}, v^{(n)}) = \eta(x^{(n)}) \) | \( W \in \mathbb{R}^{2d \times d'} \) | \( \rho(x^{(n)}) = u^{(n)} \odot (x^{(n)} + v^{(n)}) \) |
| IV   | \( (u^{(n)}, v^{(n)}) = \eta(x^{(n)}) \) | \( \tilde{W} \in \mathbb{R}^{2d \times d'} \) | \( \rho(x^{(n)}) = (u^{(n)} \odot x^{(n)}) + v^{(n)} \) |

Fig 2(f) shows the reallocated feature vectors \( \rho(x^{(n)}) \); the blue and orange dots are linearly classified. Note that we used \( C \) (\( \min = 0.0 \) and \( \max = 1.0 \)) in Eq (11). As long as the reallocated vector \( \rho \) is defined by the Hadamard product operator as in Eq (11), one can obtain the weight \( \xi^{(n)} \) in the same manner as Eq (10).

Moreover, various NNs, including RNNs and CNNs, can be used to compose the feature vector \( \varphi \) in Eq (2). The point-wise linear model enables all these NNs to explain the machine’s prediction with respect to the low-dimensional original feature vector \( x \), while the NNs can improve the prediction’s accuracy by using the high-dimensional feature vector \( \varphi \).

### Regularization

To avoid the overfitting problem, the loss functions of prediction models have the \( L_p \)-norm of the learning parameters as the regularization term. Logistic regression models generally use \( L_1 \) and \( L_2 \)-norm regularization, which are equivalent to lasso and ridge regression models, respectively [22]. From the viewpoint of the point-wise linear model, the learning parameter is \( \xi \), and the regularization terms should correspond to the \( L_1 \)-norm \( |\xi|_{L_1} \) and \( L_2 \)-norm \( |\xi|_{L_2} \). The \( L_p \) (\( p = 1, 2 \)) regularization term is given by

\[
L_p \left( \xi(x^{(n)}) \right) = \left| w \odot \eta(x^{(n)}) \right|_p. \tag{13}
\]

The above equation constrains the range (magnitude) of \( \eta(x^{(n)}) \). The \( L_p \)-norm reduces the cost of the reallocation of the original feature vector \( x^{(n)} \). It induces sparseness in the network pathway of \( \varphi \). Additionally, Eq (13) can be extended to an elastic-net regularization term as follows:

\[
L_{\text{elastic}} \left( \xi(x^{(n)}) \right) = \alpha L_1 \left( \xi(x^{(n)}) \right) + (1 - \alpha) L_2 \left( \xi(x^{(n)}) \right), \tag{14}
\]

where \( \alpha \) is a mixing parameter with \( 0 \leq \alpha \leq 1 \).

### Variants

The necessary condition for constructing a point-wise function is that the reallocation function is linear (see Table 1). These reallocation functions allow us to calculate an element-wise magnitude of the point-wise learning weight for each feature. For example, the learning weight and bias term of the type II (adaptive reallocation) function are \( w_{\mu}u^{(n)}_\mu \) and \( w_{\mu}x^{(n)}_\mu \), respectively. The functions of types I–IV have almost equal prediction abilities, as shown in Fig 3. Each panel shows the classification boundaries in feature vectors (generated by \texttt{sklearn.datasets.make_moon}). The type I (multiplicative reallocation) vector \( \rho \) is equivalent to the weight of the logistic regression-type linear models, so medical researchers familiar with logistic regression may find the properties of type I especially useful.

### 3 Experiments

To be published in PLOS ONE.
Figure 3: Classification results for each reallocation function. The dataset is sklearn.datasets.make_moon. Each panel shows the classification boundary obtained by one of the following the reallocation functions: (a) $u(n) \odot x(n)$, (b) $u(n) + x(n)$, (c) $u(n) \odot (x(n) + v(n))$, or (d) $(u(n) \odot x(n)) + v(n)$.

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