1 Introduction

Complex problems may require sophisticated, non-linear learning methods such as kernel machines or deep neural networks to achieve state-of-the-art prediction accuracies. However, high prediction accuracies are not the only objective to consider when solving problems using machine learning. Instead, particular scientific applications require some explanation of the learned prediction function. Unfortunately, most methods do not come with out-of-the-box straight-forward interpretation. Even linear prediction functions $s(x) = \sum_j \beta_j x_j$ are not straightforward to explain if features $\beta_j$ exhibit complex correlation structures.

In computational biology, positional oligomer importance matrices (POIMs) [7] address the need for interpretation of sophisticated learning machines. POIMs specifically explain the output of kernel-based learning methods acting on DNA sequences using a weighted degree string kernel [1, 5, 3]. A WD kernel breaks two discrete DNA sequences $x$ and $x'$ of length $L$ apart into all subsequences up to some length and then counts the number of matching subsequences—the so-called positional oligomers (POs). For the following considerations, let $\Sigma = \{A, C, G, T\}$ be the DNA alphabet and $X \in \Sigma^L$ a random variable over the DNA alphabet of length $L$. POIMs assign each PO $y \in \Sigma^k$, of length $k$ starting at position $j$ in $X$ with an importance score $\text{POIM}_{y,j} \propto \mathbb{E}[s(X)|X_{j:j+k} = y]$. POIMs allow visualization of each PO’s significance to the prediction function $s$. A seminal property of POIMs is that they take the overlaps of the POs at different positions and lengths into account. As visual inspecting POIMs can be tedious, [9, 8] proposed motifPOIMs, a probabilistic non-convex method to automatically extract the biological factors underlying the SVM’s prediction such as promoter elements or transcription factor binding sites—often called motifs. Unfortunately, POIMs are restricted to specific DNA applications.

As a generalization of POIMs, the feature importance ranking measure (FIRM) [10] assigns each feature $f$ with an importance score $Q_f := \sqrt{\text{Var}_Y [\mathbb{E}_X |s(X)|f(X) = Y]}$. FIRM measures the variation of the prediction function when varying a feature. If the expected value of the prediction function is not changed when varying a feature $f$, the feature is considered as unimportant. Unfortunately, FIRM is in general intractable [10].

In this paper, we propose the Measure of Feature Importance (MFI). MFI is general and can be applied to any arbitrary learning machine (including kernel machines and deep learning). MFI is intrinsically non-linear and can detect features that by itself are inconspicuous and only impact the
prediction function through their interaction with other features. Lastly, MFI can be used for both — model-based feature importance (as POIMs and FIRM) and instance-based feature importance (i.e., measuring the importance of a feature for a particular data point).

2 Methodology

In this section, we describe our proposed method — Measure of Feature Importance (MFI). MFI extends the concepts of POIM and FIRM (which are contained as special cases) to non-linear feature interactions and instance-based feature importance attribution, and it is particularly simple to apply. To distinguish between model-based and instance-based MFI, we introduce a function called “explanation mode”, which maps the sample in their respective feature space. Exemplary, for instance-based explanation, a DNA sequence would be mapped to itself, whereas the same sequence would be mapped to a POIM in case of model-based explanation.

Definition 1 (MFI and kernel MFI). Let $X$ be a random variable on a space $X$. Furthermore, let $s : X \rightarrow \mathcal{Y}$ be a prediction function (output by an arbitrary learning machine), and let $f : X \rightarrow \mathbb{R}$ be a real-valued feature. Let $\phi : X \rightarrow F$ be a function (“explanation mode”), where $F$ is an arbitrary space. Lastly, let $k : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ and $l : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ be kernel functions. Then we define:

$$MFI : S_{\phi,f}(t) := \mathbb{E}[s(X)\phi(X)|f(X) = t]$$

$$kernel\ MFI : S_{\phi,f}^+(t) = \text{Cov}[k(s(X), s(\cdot)), l(\phi(X), \phi(\cdot))|f(X) = t]$$

Table 1: Specific instantiation for MFI in terms of instance-based (ib) and model-based (mb) application, with $B \in A^k \times \{1, \ldots , L - k + 1\}$. Illustrations are given in Figure 1.

| Objects | mode | method   | $\phi$         | $f$          | $t$          |
|---------|------|----------|----------------|--------------|--------------|
| a       | Image z | ib MFI   | $\phi(X) = 1$ | $f_{i,j}(X) = X_{i,j}$ | $t = z_{i,j}$ |
| b       | Sequence z | ib MFI | $\phi(X) = 1$ | $f_{i,k}(X) = X_{i+k}$ | $t = z_{i+k}$ |
| c       | Images | mb kernel MFI | $\phi(X) = X$ | $f(X) = t$ | $const$ |
| d       | Sequences | mb kernel MFI | $\phi(X) = B$ | $f(X) = t$ | $const$ |

Figure 1: MFI Examples We consider two possible flavors of feature importance: (left) instance-based importance measures (e.g. Why is this specific example of ‘3’ classified as ‘3’ using my trained RBF-SVM classifier?); (right) model-based importance measure (e.g. Which regions are generally important for the classifier decision?).

In the following, we will explain the “explanation mode” of above definition in terms of model-based and instance-based proceed exemplary for both, sequence and image data.

2.1 Model-based MFI:

Here, the task is to globally assess what features a given (trained) learning machine regards as most significant — independent of the examples given. In the case of sequence data, we have sequences of length $L$ over the alphabet $\Sigma = \{A, C, G, T\}$, an importance map for all $k$-mers over all positions is gained by using the explanation mode $\phi : \Sigma^L \rightarrow \Sigma^{L-k+1}$, where each sequence is mapped to a sparse PWM, in which entries only indicate presence or absence of positional $k$-mers. In the case of two dimensional image data, $X \in \mathbb{R}^{d_1 \times d_2}$, where we already are in the decent visual explanation mode, $\phi(X) = X$ keeps the surroundings by mapping the data to itself. In both cases, we set $f(X) = t$, where $t = const$, which is why we can neglected it. The various case studies are summarized in Table 1 with corresponding examples shown in Figure 1 on the right.
2.2 Instance-based MFI:

Given a specific example, the task at hand is to assess why this example has been assigned this specific classifier score (or class) prediction. In the case of sequence data we compute the feature importance of any positional $k$-mer in a given sequence $g \in \Sigma^L$ by $f(X) = X_{i:j+k}$, with $t = g_{i:j+k}$. In the case of images, where $g \in \mathbb{R}^{d_1 \times d_2}$ is the image of interest and $g_{i,j}$ expose one pixel, $f(X) = X_{i,j}$ maps the random samples $X \in \mathbb{R}^{d_1 \times d_2}$ to one pixel $t = g_{i,j}$. In both cases, we set $\phi(X) = 1$, which is why we can neglect it. For examples and specific instruction see Table 1 and Figure 1 on the left.

2.3 Relation to Hilbert-Schmidt Independence Criterion

In 2005, the Hilbert-Schmidt independence criterion [2] (HSIC) was proposed as a kernel-based methodology to measure the independence of two distinct variables $X$ and $Y$:

$$\text{HSIC}(X, Y) = \|C_{XY}\|^2 = E[k(X, X')l(Y, Y')] - 2E[E_X[k(X, X')|E_Y[l(Y, Y')]] + E[k(X, X')|E[Y, Y']]]$$

where $k$ and $l$ are reproducing kernels and $C_{XY}$ is the cross-covariance operator. We have the following interesting relation of MFI to HSIC.

**Lemma 1** (Relation of Kernel MFI to HSIC). Given the kernel MFI of Definition 1 $S_{\phi, f}^{+}$, then $S_{\phi, f}^{+} = \text{Cov}[k(s(X), s(\cdot)), l(\phi(X), \phi(\cdot))]f(X) = t$ and the corresponding Hilbert-Schmidt Independence Criterion becomes: $\text{HSIC}(S_{\phi, f}, Y, \mathbb{R}) = \|S_{\phi, f}^{+}\|^2 = tr(KL)$.

The relation to HSIC provides us with a practical tool to assess non-linear feature importances as defined in kernel MFI in Definition 1. In order to make this approach practically suitable, we resort to sampling as an inference method. To this end, let $Z \subset \mathcal{X}$ be a subset of $\mathcal{X}$ containing $n = |Z|$ samples. Then Eq. (1) can be approximated by $\hat{S}_{\phi, f}(t) := \frac{1}{|Z_{(f(t) = t)}|} \sum_{z \in Z_{(f(t) = t)}} s(z) \phi(z) 1_{f(z) = t} - \mu_X \mu_\phi$ with $\mu_\phi = \frac{1}{|Z_{(f(t) = t)}|} \sum_{z \in Z_{(f(t) = t)}} \phi(z)$ and $\mu_X = \frac{1}{|Z_{(f(t) = t)}|} \sum_{z \in Z_{(f(t) = t)}} s(z)$. Hence, when number of samples $|Z| \to \infty$, then $\hat{S}_{\phi, f} \to S_{\phi, f}$. A corresponding sampling scheme is also available for kernel MFI.

3 Empirical Evaluation

In this section, we evaluate the proposed method empirically regarding its ability to explain the relevance of features for model- and instance-based explanation models. Although our method can be applied to any learning machines, we focus in the experiments on support vector machines (SVMs) using a Gaussian kernel function and convolutional neural networks (CNNs).

3.1 Experimental setup

For validation, we follow the Most Relevant First (MoRF) strategy [4] and successively calculate the classifier performance while blurring pixels a) with descending relevance (i.e., computed by our proposed method) and b) randomly. The idea is that blurring pixels with high relevance will influence the classifier decision and thus drop its performance faster than blurring randomly chosen pixels would do. In the following, we evaluate our proposed method on the USPS data set, using a SVM with an RBF kernel and a CNN with following architecture: a 2D convolution layer with 10 tanh-filters of size 8x4, a max-pool layer of size=2, a dense-layer with 100 ReLUs, a dense layer with 2 softmax units. For all experiments, we used a sample size of 1000 samples, which was considered as suitable trade-off between runtime and accuracy.
3.2 Results

To find a suitable trade-off between runtime and accuracy, we evaluate runtime and convergence behavior (in terms of the Frobenius distance of two consecutive results) for increasing numbers of samples. From the results, shown in Figure 2, we observe that the Frobenius distance (green curve) converges to zero already for small sample sizes (215 samples). Unfortunately, runtime grows very fast (almost exponentially) showing the boundaries of our method. Hence, a good trade-off between runtime and accuracy would be any sample size between 500 and 2000 in this experiment. For the following experiments we used a sample size of 1000.

Model-Based Feature Importance The results are shown in Figure 3. We observe that for both, SVM and CNN, the pixel bridge that changes the digit three to the digit eight is of high importance. In Figure 3 (c) and (d) the classifier performance for increasing amount of blurring pixels in terms of MoRF as explained above is shown. Compared to a random pixel blurring, we can clearly observe that the performance drops significantly faster when blurring the most important pixels (as found by our proposed kernel MFI method).

Instance-Based Feature Importances For the pixel-wise explanation experiment, an SVM with an RBF kernel was trained on the USPS training data set. From Figure 4, we observe that the pixels building the vertical connection from a three to an eight have a strong discriminative evidence. If these positions are left blank, the image is classified as three, which, in case of the last three images leads to mis-classifications.

For the nucleotide-wise explanation experiment, an SVM with an WD kernel was trained on a synthetic training data set. We inserted two motifs in the positive class (GGCCGTAAC at position 11 and TTTCACGTGA at position 24). From Figure 5, we observe that the nucleotides building the two patterns, which we inserted in the positive sequences have strong discriminative evidence. If the discriminative patterns are too noisy, the sequences are assumed to stem from the negative class, which, in case of the false negative (FN) example leads to mis-classifications. If only one of the two patterns was inserted, the classifier gives high evidence to the single pattern and assigns the wrong label.

Figure 3: Results are shown for the USPS data set using kernel MFI for SVM (a) and CNN (b), where the most important pixels found by kernel MFI are embedded in the mean picture of digit three. Figure (c) and (d) show the classifier performance loss when successively blurring the pixel regarding their relevance found by kernel MFI compared to a random pixel blurring.

Figure 4: Instance-based explanation of the SVM decision for five USPS test data images. The highlighted pixels are informative for the individual SVM decisions (plotted at the image top) – only the first two images were correctly classified.

Figure 5: Instance-based feature importances experiment. The highlighted nucleotides are informative for the SVM decision for four test sequences that have been correctly (TN and TP) and incorrectly (FP and FN) classified.
4 Conclusion & Outlook

By this work, we contributed to opening the black box of learning machines. Building up on POIMs and FIRM, we proposed MFI, which is a general measure of feature importance that is applicable to arbitrary learning machines. MFI can be used for both for a general explanation of the prediction model and for a data instance specific explanation. As a nonlinear measure, MFI can detect features that exhibit their importance only through interactions with other features. Experiments on artificially generated splice-site sequence data as well as real-world image data demonstrate the properties and benefits of our approach.

While in the present work we have focused images and sequences, the framework allows us to explain arbitrary data sources. In future research, we would like to study further applications (e.g., involving trees, graphs, etc), including wind turbine anomaly detection, as well as we want to investigate advanced sampling techniques from probabilistic machine learning that may lead to faster convergence.

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