Explainable Predictive Process Monitoring: Evaluation Metrics and Guidelines for Process Outcome Prediction

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Abstract—Although a recent shift has been made in the field of predictive process monitoring to use models from the explainable artificial intelligence field, the evaluation still occurs mainly through performance-based metrics, thus not accounting for the actionability and implications of the explanations. In this paper, we define explainability through the interpretability of the explanations and the faithfulness of the explainability model in the field of process outcome prediction. The introduced properties are analysed along the event, case, and control flow perspective which are typical for a process-based analysis. This allows comparing inherently created explanations with post-hoc explanations. We benchmark seven classifiers on thirteen real-life events logs, and these cover a range of transparent and non-transparent machine learning and deep learning models, further complemented with explainability techniques. Next, this paper contributes a set of guidelines named X-MOP which allows selecting the appropriate model based on the event log specifications, by providing insight into how the varying preprocessing, model complexity and explainability techniques typical in process outcome prediction influence the explainability of the model.

Index Terms—Explainable Artificial Intelligence, Predictive Process Monitoring, Interpretability, Faithfulness, Deep Learning, Machine Learning

1 INTRODUCTION

The analysis of processes through data-driven approaches is labelled as process mining [1] and has seen a strong uptake over the past two decades. Among the wide range of its techniques, the focus of this study lies on predictive process monitoring [2], the umbrella term geared towards predictive activities. It allows identifying process-related trends regarding particular outcomes (e.g., will customers be awarded credit?), impeding bottlenecks, and whether particular activities will occur in the future. In the case of Outcome-Oriented Predictive Process Monitoring (OOPPM), the concrete objective is to predict the outcome of an incoming, incomplete process case, for which the primordial goal is to do so as accurately as possible. Here, an often anticipated trend is to increase the predictive performance by focusing on representation learning [3], [4], [5], or on the introduction of computationally complex models such as ensemble models [2], [3], deep neural networks [6], [7], [8], and many more algorithms [9]. Nonetheless, the inability to link the output back to the original inputs consequently inhibits to understand the model’s behaviour. In response to this, the field of eXplainable Artificial Intelligence (XAI) focuses on gaining insights into how and why certain predictions in complex structures were made, while trying to maintain the predictive performance of these highly performant models [10]. Many XAI proponents state that trying to explain these complex models come with a loss of faithfulness [11], considering the fact that the relationship between input and output can only be approximated [11], [12], [13]. Nonetheless, the use of increasingly complex models has been widely adopted in high stake decision-making processes throughout society [14].

This paper identifies three main issues that arise at the intersection of OOPPM and XAI. First, the existing OOPPM research is constrained to the computational aspects while neglecting the interpretation, actionability, and implications of the results. In addition, the existing evaluation metrics are not adapted to a process-based analysis (i.e., do not take into account the different perspectives of a process-based analysis) or are not model agnostic (i.e., metrics are dependent on model parameters), making them not suitable for evaluation purposes. Second, recent literature pointed out that the post-hoc explainability techniques should uncover, apart from an interpretable explanation, the true reasons for model predictions [12], [13], [15]. Hence, a more comprehensive study about the faithfulness and interpretability of XAI techniques in OOPPM is missing, which impedes the selection of the most appropriate setting of preprocessing techniques, predictive algorithms and explainability models to achieve an interpretable outcome. Third, the main focus of this field is to verify its conformance with respect to the business requirements and goals [1], [16], [17]. Moreover, there is need for a set of guidelines towards obtaining faithful and interpretable explanations in the context of business process monitoring.

This paper tackles these issues through three contributions. First, we establish a comprehensive basis for XAI in OOPPM by introducing model-agnostic evaluation metrics based on the properties interpretability and faithfulness and adapt these along the event, case, and control flow.
In [28] and [29], they use a Bidirectional LSTM, where Short-Term Memory (LSTM) model with the use of SHAP attributes in the different steps of the process in a Long developments in a deep learning context [26], [27], [28], [29], Model-Agnostic Explanations (LIME) [25], with similar de-
Additive exPlanations (SHAP) [24] or Local Interpretable top of machine learning models [22], [23] such as SHapley papers have already suggested explainability techniques on hoc techniques. In predictive process monitoring, several generates explanations for the black box model using post-
explainability-performance trade-off [10]. The first trend two different trends based on how they deal with the of movement around explainability in predictive process monitoring.  
Next, a definition for explainability is given, together with the introduced metrics in Section 4. The benchmark study and implementation details can be found in Section 5.  
Next, we clarify the research questions in Subsection 5.1. In Section 6 the insights obtained from the research questions are incorporated into the framework of guidelines named X-MOP. Finally, the results and obtained insights are con-
cluded in Section 7.

2 Related Work and Motivation

Predictive process monitoring is concerned with providing insights about the business processes of modern organiza-
tions. Most predictive efforts are primarily driven by using machine learning models such as XGBoost [2], [19], random forest [2], [6], support vector machines [2], [6] or logistic regression (LR) [2], with recent works showing interest in applying deep learning models [6], [20], [21]. Nonetheless, the lack of transparency of these sophisticated models prohibits the ability to understand the rationale of the decision-making process.

Over the last two years, there has also been a lot of movement around explainability in predictive process monitoring. The different works are often divided into two different trends based on how they deal with the explainability-performance trade-off [10]. The first trend generates explanations for the black box model using post-hoc techniques. In predictive process monitoring, several papers have already suggested explainability techniques on top of machine learning models [22], [23] such as SHapley Additive exPlanations (SHAP) [24] or Local Interpretable Model-Agnostic Explanations (LIME) [25], with similar developments in a deep learning context [26], [27], [28], [29], [30]. As an example, [26] visualizes the influence of certain attributes in the different steps of the process in a Long Short-Term Memory (LSTM) model with the use of SHAP values, while Mehdiyev [27] focuses on creating local post-hoc explanations with the use of a surrogate decision tree. In [28] and [29], they use a Bidirectional LSTM, where after the hidden states of the time steps of both RNNs are concatenated. After this, a context vector is learnt that takes the different time steps into account. Finally, [30] visualizes the impact of the activities on the predictions with the use of gated graph neural networks. The benchmark study of [23] compares different explainability models and evaluates the settings with properties unrelated to explainability, such as stability and duration of execution.

The second trend introduces interpretable models instead of trying to break open these black box models, stating that there are alternative models that yield better explainability-performance trade-offs. In [17], a set of fuzzy rules are learnt from neural networks. Here, the relationship between inputs and output is determined by a set of IF-THEN rules. Nonetheless, this approach requires domain knowledge in order to bin the attributes into different interpretable terms. Next, a Bayesian network is used in [9] for next event and suffix prediction. Even though the causal relationships are inferred from historical data, it relies on domain knowledge assumptions [10]. Finally, [18] introduces two inherently interpretable models to OOPPM, i.e., Logit Leaf Model (LLM) and Generalized Logistic Rule Model (GLRM), both drawn from XAI literature and adapted to the OOPPM case.

In the field of XAI, a wide range of works have already evaluated these different models with predictive performance-based metrics [6], [21] or with quantitative metrics to assess the quality of the explanation methods [13], [31], [32]. Nonetheless, these metrics do not take into account the different perspectives that are typical of a process-based analysis. As an example, Islam [32] created a metric for explainability based on the human-friendly properties that define the concept explainability, while [31] introduces a metric based on three different properties that define the model complexity. Likewise, [13] introduced quantitative metrics for different kinds of explanations types, based on the identified properties for explainability. Additionally, none of the metrics evaluate the faithfulness of the explainability model. An initial attempt was made by Nguyen [33], advising the use of mutual information to describe the faithfulness of explanation methods on top of deep learning models, but this metric is not model-agnostic (i.e., can not be calculated for all explainability models). Next, the work of Jain and Wallace [34] states that the learned attention weights are uncorrelated with the gradient-based attribute importance, even though they mimic the predictions rather accurately. Similarly, Velmurugan [19] used a perturbation-based technique to investigate the faithfulness of SHAP and LIME in the field of OOPPM, and the results report low-to-moderate faithfulness scores.

A comprehensive study about the (un)faithfulness in OOPPM is missing due to a number of reasons. The accuracy by which these post-hoc explanations reflect the effective model behaviour of the predictive model is often inadequate in terms of attribute space [11], [18]. Moreover, work from related field show that there are substantial problems with the use of post-hoc explainability methods. First, the findings of [15] show that the importance ranking of the attributes made by the attention scores is not faithful to the model decisions (i.e., what the model perceived as important). Second, demonstrates that there is a non-monotonic relationship between the SHAP values and the
predictive performance \cite{35}.

The above works indicate the need for model-agnostic explainability metrics that are adapted to OOPPM. Furthermore, there is a growing need to evaluate the faithfulness of (post-hoc) explainability methods. Therefore, these metrics should include both the faithfulness of the explainability technique and interpretability of the explanations. These domain-specific metrics can guide practitioners to select the best model for the task at hand \cite{35} and would reduce the scope of research for human-based studies by reducing the financial and time costs of such experiments. There is a notable void in the OOPPM literature in this respect, which this paper will address through both introducing the notions of interpretability, faithfulness, and a OOPPM-specific set of guidelines.

3 Preliminaries

This section first describes the different terminology inherited from the XAI field, followed by the preliminary steps needed for predictive process monitoring purposes.

3.1 The different XAI nomenclatures

Task model. As mentioned in Section 1, the task model is defined by several studies as the model that generates the predictions \cite{11, 12}.

Transparency. Recent literature describes transparency as the opposite of blackbox-ness \cite{10}. Furthermore, a transparent model (also referred to as an interpretable model) is a task model that is able to generate its own explanations, where the black box model requires the need of an additional explainability model.

Interpretability. Originally described as comprehensibility in \cite{10}, the interpretability is the ability to provide an explanation that consists out of single chunks of information, preferably in a human understandable fashion. Furthermore, it is often quantified by the related concept of model complexity \cite{10, 31}.

Explainability model. The explainability model is the model that generates the explanations for the predictions made by the task model. This means that a transparent model is technically also an explainability model, while the explainability model of a black box model can be, e.g., a surrogate model \cite{27}, an attention layer \cite{29} or SHAP values \cite{24}. Previous research has mostly referred to this as post-hoc explanations \cite{10, 12}, or post-hoc interpretations \cite{31}. Here, the term explainability model is used to indicate that the post-hoc explainability techniques should be both interpretable and faithful (see infra).

Faithfulness. The faithfulness of an explainability model can be considered as the accuracy by which the explainability model accurately mimics the behaviour of the task model (and not the predictions of the task model), as similar predictions do not ensure that it correctly mimicked the behaviour of the task model \cite{11}.

Explainability. Even though often used interchangeably \cite{10}, interpretability and explainability differ significantly due to the fact that an interpretable explanation is not always faithful. To emphasize, a simple explanation generated for a rain forecast prediction could be: ‘if the grass is green, it will rain’, which is easy to interpret, but unfaithful. The necessity to distinguish between faithfulness and interpretability has already been pointed out by prior research \cite{12, 13}.

3.2 OOPPM setup

OOPPM relies on the use of historic process data recorded in an event log, which is a list of traces which represent the enactment of a process for a particular case within an information system \cite{37}. Moreover, a trace is considered a sequence of timestamped events generated by executing a particular activity in the process. An event is a tuple of \( d \) attributes \( x^\prime_{j, i,j} \in \{1,...,d\} \) such as an activity name, Case ID, timestamp, and so on. In the situation of a loan application process, each event records the occurrence of an activity (i.e. control flow attribute) up until the loan request is either accepted or rejected, with each activity having complementary case and event attributes. These case attributes remain unchanged (i.e. static) within each case, while the event attributes have varying values (i.e. dynamic) for every event. This means that an event has three different attribute types: case, event and control flow attributes.

The first transformation step extracts (trace) prefixes from the completed cases to be able to learn, preferably incrementally (over time), from the development of the traces. To this end, a prefix log is typically derived, which is the extracted event log that contains all the prefixes of each case in the original event log. Next, trace cutting is performed in \cite{2}, i.e. they limit the prefix length for computational reasons.

The second data transformation step describes the encoding mechanism that enables the user to work with a varying amount of attributes, since each trace can have a different length. In the work of van Dongen \cite{35}, the focus is on the order and execution of the activity in the trace (i.e. control flow encoding), with further research in predictive monitoring \cite{2, 4, 39} advising to expand the attribute space with other event and case attributes. An often used encoding mechanism is the aggregation encoding technique \cite{5}. First, the categorical static attributes are one-hot encoded, which means that each categorical static attribute \( x^\prime_{j} \) results in a number of transformed attributes based on the unique attribute values \( \theta(x^\prime_{j}) \), with \( \theta(x^\prime_{j}) = \{x^\prime_{i,j_i} \mid i \in \{1,...,n\} \} \). The numeric static attributes remain unchanged. Second, the dynamic numeric attributes are replaced by their summary statistics \( \min, \max, \text{mean}, \text{sum} \) and \( \text{std} \). The last transformation step relates to the dynamic categorical attributes, where the frequency of occurrence of an attribute value in a prefix is the value for the new attribute. To overcome the obvious drawbacks of the lossy aggregation encoding, the idea of index encoding \cite{2, 4} is to use all possible information in the trace, including the order of the trace. First, a categorical event attribute generates a number of attributes with a factor similar to the number of attribute values multiplied with the prefix length. Note that only for the activity values that actually happened (i.e. visible in the event log), a new index is created. Second, the amount of case attributes remain unchanged compared to the aggregation encoding due to their static nature. This way, a lossless encoding of the trace is achieved, which
means that it is possible to completely recover the original trace based on its attribute vector. By contrast, the use of the above encoding mechanism in step-based models such as recurrent neural networks becomes superfluous given their sequential setup. To exploit this efficiently, a low-dimensional representation of discrete attributes in the form of embeddings is an often performed encoding technique [6]. This mapping transforms the categorical attribute to a vector of continuous numbers, similarly to how one-hot encoding works. Nonetheless, the latter ignores the similarity between the obtained vectors. In the next part of this paper, the attributes $x_{ij}$ are the resulting attributes after the data transformation steps, performed on the train event log. Consequently, the value for prefix $i, i \in \{1, \ldots, n\}$ on attribute $x_{ij}, j \in \{1, \ldots, p\}$ is denoted by $x_{i,j}$.

A third data transformation step is referred to as trace bucketing, commonly used to support the discovery of heterogeneous segments in the data [2], [4], [10], while creating separate models for each of them. Techniques such as K-Nearest Neighbours [9] or K-Means clustering measure the (dis)similarity between traces depending on the parameter K. The prefix bucketing technique [4] creates different buckets for the prefixes of different lengths, while the state-based bucketing technique [41] creates a different model for each different decision point within the process model. Although these bucketing techniques can effectively diminish the runtime performance [2], they do not necessarily result in an intuitive or interpretable outcome. E.g., clustering techniques can base their grouping on a high number of dimensions that are not interpretable. Furthermore, there is no guarantee that the use of a bucketing technique will effectively improve performance. These insights were obtained and tested in [5].

After the data transformation steps, the transformed event log is split into a train and test event log, where the former is used to create a task model to predict the dependent variable based on independent attributes. Moreover, the prediction for prefix trace $i$ is denoted as $\hat{y}_i = F(x_{i,1}, \ldots, x_{i,p})$. The final step is to interpret the predictions made by the task model. In the one hand, in a transparent model indicate the importances of the different dimensions that are not interpretable. Furthermore, there is no guarantee that the use of a bucketing technique will effectively improve performance. These insights were obtained and tested in [6].

4 Explainability in OOPPM

The separation of explainability into interpretability and faithfulness stems from [12] and [13], and is adapted in this paper to obtain model-agnostic metrics suitable for a process-based analysis. As a result, the combination of interpretability of explanations and faithfulness of explainability model allows quantifying and thus evaluating explainability in the field of OOPPM.

To determine the interpretability of an explanation in the context of OOPPM, it is necessary to divide the attributes into the different attribute type (see Section 3), allowing the metrics to take into account the process-based perspectives. Furthermore, an interpretable model is different from the interpretability of the explanation. An interpretable model (e.g., a logistic regression model) that creates its own explanations based on more than 500 attributes [42], has a low value for interpretability of explanation. In the XAI literature, the explainability-accuracy trade-off compares the model interpretability (and not interpretability of explanation) with the model accuracy, assuming that it is required to strike a balance between either simple models (e.g., linear regression) or models using complex inference structures (e.g., neural networks). By contrast, this paper investigates whether the interpretability of an explanation is also in trade-off with the predictive accuracy. In this sense, a non-interpretable deep neural network can have higher interpretability of explanations compared to a logistic regression model.

In the following subsection, four different explainability metrics are adapted to and interpreted considering the OOPPM context. Figure 2 describes the pipeline to calculate the two interpretability and two faithfulness metrics.

4.1 Quantitative Metrics

 Parsimony ($C$) is a property of interpretability [42] that represents the complexity of a model [12], an often used metric for linear regression models. This can be seen as the number of attributes with non-zero weights e.g., non-zero linear regression coefficients, in other cases the non-zero weights provided by the post-hoc attribute importance that needs to be calculated post-hoc.

We adapt this metric to take into account the different perspectives of a process-based analysis by determining the parsimony for each attribute type $t$. This metric is quantified by the number of attributes of attribute type $t$ in the resulting model. The parsimony of the total model $C_F$ is equal to the sum of the values for parsimony of the attribute types $t$. Moreover, a parsimonious (i.e. simple) model corresponds to a low value for $C_F = C_{\text{event}} + C_{\text{case}} + C_{\text{control}}$.

Assume attribute $x_{j,k}$ with $w_{j,k}$ the weight of an attribute $x_{j,j} \in \{1, \ldots, p\}$ in the model $F$, with attribute type $t \in \{1, \ldots, k\}$. Then, the total parsimony $C_F$ is calculated as follows:

$$C_F = \sum_{k=1}^{t} \sum_{j=1}^{p} C(x_{j,k})$$

with

$$C(x_{j,k}) = \begin{cases} 1, & \text{if } w_{j,k} > 0, \\ 0, & \text{otherwise}. \end{cases}$$

Since the focus is on the interpretability of the explanation, we define the parsimony of the model as a property for the interpretability of an explanation rather than a property for model interpretability.

Functional Complexity (FC) is a measure for model complexity in line with other FC calculations such as [31] and is made suitable for OOPPM data. In addition, [43]
states that small random perturbations to the test images can drastically change the generated explanations, without the predicted label being flipped. For this, we adapt the metric further by investigating how many different predictions there would be when permuting the attribute values of an attribute type, and consequently measures how strongly the explanations depend on that attribute type. This permutation-based metric is consequently used to retrieve the dependency of the attribute types (i.e., event/case/control flow) on the explanations by investigating how much percent of the predictions are flipped. In Algorithm 1, the pseudocode for the proposed FC algorithm is given, and how the different permutations are made in order to obtain the FC values for the different attribute types.

Algorithm 1 Functional Complexity

Require: \(x_1, \ldots, x_p, \ldots, x_{m,1}, \ldots, x_{m,p}\)
Ensure: \(FC_{event}, FC_{case}, FC_{control}\)

\begin{align*}
\text{Attribute types} & \leftarrow \{\text{event, case, control}\}, FC_{event} \leftarrow 0, FC_{case} \leftarrow 0, FC_{control} \leftarrow 0, z \leftarrow ()
\end{align*}

\begin{align*}
\text{Test} & \leftarrow (x_1, \ldots, x_p, \ldots, x_{m,1}, \ldots, x_{m,p}) \\
\text{To make the pseudocode simpler}
\end{align*}

3: \text{for } t \in \text{Attribute types do}

\begin{align*}
\text{Test}_{copy} & \leftarrow \text{Copy} (\text{Test}) \quad \text{copies the test data for each attribute type } t \\
\text{for } j \in \text{Attributes do} & \quad \text{take only the attributes of type } t \\
\text{NewValues} & \leftarrow () \quad \text{all the unique attribute values of that attribute}
\end{align*}

6: \text{for } i \in \text{Instances do}

\begin{align*}
\text{Value} & \leftarrow \text{Test}[i, j] \quad \text{the current attribute value of instance } i \\
\text{if } \text{length}(z^*) \leq 1 & \text{then} \\
\text{NewValues}[i, j] & \leftarrow \text{Value} \quad \text{for static attributes}
\end{align*}

12: \text{else}

\begin{align*}
\text{NewValues}[i, j] & \leftarrow \text{Random}(z^*) \quad \text{take a random value}
\end{align*}

15: \text{Test}_{copy}[i, j] \leftarrow \text{NewValues} \quad \text{replace with the permuted attribute values}

16: \text{predictions after permuting attributes of type } t

18: \text{FC}_t \leftarrow \frac{\text{distance}(g^*, g^t)}{n} \quad \text{a different FC for each attribute type } t

Assume \(g^* = F(x_1, j, \ldots, x_i, j, \ldots, x_{t, j+k}, \ldots, x_{m,p})\) as the prediction after permutation for attribute type \(t\), where \(x_i, j, \ldots, x_{t, j+k}\) are the permuted attribute values of the attribute \(x_j, \ldots, x_{j+k}\) of the test instance \(i\). The algorithm starts by selecting the attributes of a certain attribute type (lines 3-5), with the attribute value of instance \(i\) for attribute \(x_j\) removed from the set of permuted values in line 10. Next, the functional complexity of an attribute type is calculated as the amount of prediction changes before (line 16) and after (line 17) permuting all the attributes of an attribute type \(t\), divided by the number of instances. Finally, the Hamming Distance (line 18) is used as the distance measure between the different prediction vectors, where a low value for \(FC_t\) means that the predictions are created seemingly independently of this attribute type and should therefore not be regarded as an important attribute type when interpreting the explanations.

Monotonicity \((M)\) is a measure for the faithfulness of an explainability method and is quantified with the use of the non-parametric Spearman’s correlation coefficient \([33]\). If the model inherently creates its own explanations (e.g., logistic regression coefficients), then the monotonicity is ensured (i.e. \(M = 1\)) by design \([11]\).

The original metric \([33]\) is model dependent on a neural network model. Consequently, this paper adapted the metric to make it model agnostic by evaluating how faithful the attribute importance ranking of the explainability model is to the ranking made by the task model. Furthermore, this metric does not make a distinction between the different attribute types, as the focus is on the relative ranking of the attributes in general. For a post-hoc explainability model, we quantify the monotonicity by the non-parametric Spearman’s correlation coefficient between the ranking of the attributes by the task model and the ranking by the explainability model. The monotonicity is defined as:

\[
M = \rho (w_a, w_e)
\]

with \(w_a = w_{a, 1}, \ldots, w_{a, p}\) the attribute weights of the task model and \(w_e = w_{e, 1}, \ldots, w_{e, p}\) the weights of the explainability model. This correlation coefficient takes a value between \([-1, 1]\) and describes the association of rank. A perfectly faithful model has a correlation coefficient of +1, where a loss in faithfulness corresponds with a value closer to 0. Consequently, a negative value corresponds to a negative rank association between the two attribute importance weights.

Level Of Disagreement (LOD@10) \([14]\) is a metric of faithfulness and originally computes the percentage of similar predictions between the task model and post-hoc explanations.

In the field of predictive process monitoring, it is useful to know the importance of the attribute types, as the obtained insights are relevant in order to improve the early prediction problem \([2]\). In this paper, the LOD@10 therefore investigates whether the task model and the explainability model focused on the same attribute type. The LOD@10, different from monotonicity, neglects the ranking of the attributes but only looks at the relative frequency of the attribute types in the top 10 most important attributes. For this, the metric is quantified with the Euclidean Distance between the relative frequency of top ten attributes of the task model \(#_{a,k}\) and the explainability model \(#_{e}\).

\[
\text{LOD@10} = d \left( \#_{a,*}, \#_{e} \right) = \sqrt{\sum_{k=1}^{t} \left( \#_{a,k} - \#_{e,k} \right)^2}
\]

and

\[
\begin{align*}
\sum_{k=1}^{t} \#_{a,k} = 10 & \quad \text{with } t \in \{1 \ldots k\} \\
\sum_{k=1}^{t} \#_{e,k} = 10 & \quad \text{with } t \in \{1 \ldots k\}
\end{align*}
\]

This metric is introduced to take into account that the number of attributes used in the task model has a negative influence on the monotonicity value. Furthermore, a high value for this LOD@10 metric indicates that the explainability model focused on rather different attribute types, which
impairs the faithfulness of the explainability model.

5 BENCHMARK STUDY

In this section, a detailed build-up to the research questions related to the interpretability and faithfulness of OOPPM models is provided. Next, the different event logs and their specifications are described, followed by a description of the benchmark models and explainability techniques often used for OOPPM purposes. Finally, the hyper optimization settings and implementation details of the different setups are given.

5.1 Research Questions

The research questions are aimed to investigate the influence of the most important steps in an OOPPM context on the explainability metrics from Section 4.1 in order to establish a set of guidelines to obtain accurate and explainable OOPPM solutions. For this, an experimental pipeline similar to the benchmark studies of [2] and [6] and extended with an XAI dimension (see Figure 2 for an overview) is used.

The first research question RQ1 aims to uncover the influence of the sequence encoding techniques (see Figure 2) on the properties of explainability in OOPPM. The choice of the encoding is an integral part of transforming process data and can have a detrimental effect on the metrics (e.g., higher $C_P$) as the index encoding creates a high-dimensional feature space (see Section 5). Nonetheless, the index encoding can be preferred over its lossy variant, the aggregation encoding, as there is no loss in information (higher expected $M$).

The second research question RQ2 discusses the influence of model complexity (see Figure 2) and aims to assess whether the deep learning model focus more on the control flow perspective (i.e. higher $C_{control}$) compared to the traditional cross-sectional statistical and machine learning models, as their sequential architecture is more tailored towards modelling time-dependent and sequential data tasks without such aggregation.

The next three research questions evaluate the different classifiers (see Figure 2). RQ3 investigates whether the previously established higher performance of the deep learning models [6] comes at the cost of interpretability and/or faithfulness. Next, this study compares the interpretable LLM model, introduced in [18], as an alternative to the bucketing technique (see Section 3) in conjunction with the LR model. In research question RQ4, the LLM model is relatively compared to the LR model based on the performance and four explainability metrics. Finally, transparent models (i.e. model that are faithful by design) typically underperform compared to the black box models in the case of sequential and high-dimensional data [6], which is evaluated with the use of research question RQ5.

The next two research questions RQ6 and RQ7 are based on how the explanations (see Figure 2) are generated, and describe the interpretability-accuracy trade-off in OOPPM. Here, the ranking of attribute types by the parsimony and the functional complexity are relatively compared. Although both metrics are a measure for model complexity, the parsimony evaluates the importance of the attribute types as perceived by the task model, while the functional complexity is the importance of the attribute types assessed on the test data. Finally, the faithfulness of the post-hoc explanations (i.e. SHAP values) is compared with the attention-based explanations that are technically calculated during the fitting of the task model. Moreover, it is implicitly assumed that the faithfulness of the latter should be higher compared to the SHAP values. This leads to the research question RQ8. The final research question RQ9 compares the monotonicity with the LOD@10 values. The monotonicity evaluates the importance ranking of all the attributes, while the LOD@10 investigate the difference in importance of the attribute types in the top 10 most influential attributes for the task model and the explainability model. Moreover, a high value for monotonicity (i.e. the model had an overall good idea of the importance ranking) can be related to a high value for LOD@10 (the model focused on a different type of attribute in the top 10 attributes).

RQ1. What is the influence of the encoding mechanism on the interpretability of the explanations and faithfulness of the explainability model?

RQ2. Do deep learning models extract more information from the sequential, control flow perspective compared to the other models which are conceived for tabular data?

RQ3. Does the previously established outperforming of the deep learning models come at the expense of the interpretability and faithfulness?

RQ4. Does the LLM model outperform the logistic regression model?

RQ5. Are transparent models capable of attaining the performance level of the black box models in the field of OOPPM?

RQ6. Is the relative ranking of parsimony values similar to the ranking of the functional complexity values?

RQ7. Does the interpretability-accuracy trade-off hold in the field of OOPPM?

RQ8. Are the explanations generated by post-hoc explainability techniques less faithful compared to the explanations that contribute to the predictions of the black box model but are typically calculated afterwards?

RQ9. Is an explainability model with a low monotonicity value always associated with a high LOD@10 value?

5.2 Event logs

This study is based on four different real-life event logs that can be found at the website of 4TU Centre for Research
Data and are often used in the field of OOPPM [2], [6], [27], [28], [30]. These event logs are split with Linear Temporal Logic (LTL) rules as defined in [2] to obtain objectives for the process. Moreover, the event log is split based on the labelling functions defined by the four LTL rules, therefore creating four different binary prediction tasks. The event log specifications are defined in Table 2.

The first event log, BPIC2011, describes the medical history of patients from the Gynaecology department of a Dutch Academic hospital. The applied procedures and treatments of the different cases represent the activities in this event log, with the label being either true or false if the LTL rule is violated or not, respectively. The four different LTL rules to generate the event logs: bpic2011(1), bpic2011(2), bpic2011(3) and bpic2011(4), are described in [2]. Next, similar trace prefixing and cutting preprocessing steps are performed as in [2].

The BPIC2015 event log assembles events pertaining to the building permit application process from five Dutch municipalities. A single LTL rule is applied on the event log and split for each of the five municipalities. The LTL rule defines that a certain activity must always be followed by (and not the other way around), where the latter activity has to always be present in the trace if the former was. No trace cutting was performed on this event log.

The sepsis cases event log contain the discharge information of patients with symptoms of sepsis in a Dutch hospital, starting from the admission in the emergency room until the discharge of the patient. Here, the labelling is performed based on the discharge of the patient instead of LTL rules [2]. In Production, the last event log contains information about the activities in a manufacturing process, together with the workers and/or machines of the production of the items itself. The labelling function is based on whether the number of work orders rejected is larger than zero or not.

5.3 Benchmark models and explainability models

The wide variety of classifiers and explainability models is depicted in Figure 2 and are chosen based on their frequent presence in other studies such as [2], [6], [26], [29]. The first model is the logistic regression model, an often used interpretable predictive technique to model the probability of a discrete variable. The two advanced logistic regression models, LLM and GLRM, are interpretable models that are introduced in [18] in the field of OOPPM. The former clusters the data with a decision tree and builds linear models in the leave nodes. The latter creates binary rules with a generalized logistic rule model. In conclusion, the former tree models generate their own explanations.

The next two models are ensemble machine learning models, i.e. XGBoost (XGB) [45] and Random Forest (RF) [46], which are not interpretable models, as the inherent complexity is what bestows their predictive abilities. In the XGB model, weak learners are iteratively improved to a final strong learner by incorporating the loss function of the previous weak learner(s). On the other hand, the RF trains a number of decision trees on various subsets of the data. Different to XGB, the voting scheme is based on the majority votes of predictions. By contrast to the transparent models, ensemble methods require an explainability model. For this, the explanations for the ensemble methods are created with SHAP values, which are calculations for each instance-attribute combination based on coalitional game theory. Here, a prediction is explained by assuming that each attribute value is a player in a game, where the prediction is the payout. This model-agnostic technique tells how to distribute the payout among the attributes, as the SHAP values are the average marginal contribution of an attribute value across all possible coalitions.

Next, two different neural network models are used. The first model is a recurrent neural network with Long Short-Term Memory (LSTM), often used for OOPPM [6], [20], [25], [28] with the long-term relations and dependencies encoded.
in the cell state vectors, designed to solve the vanishing gradient problem. The advantage of LSTM over classical machine learning models lies in the ability to model time-dependent and sequential data tasks, where the categorical values are encoded in embeddings. The second model is a Convolutional Neural Network (CNN) which is a deep-forward artificial neural network with information flow starting from the input layers, through the hidden layers, until the output layer (therefore only in one direction). To the best of our knowledge, this has only been implemented by [47] for OOPPM, but is incorporated in this study due to the frequent use in related fields such as next activity prediction [48], [49]. Similar to the ensemble methods, the internal representation of a deep neural network (LSTM and CNN), does not allow for inherent explanations of predictions. The use of attention layers is a model-specific post-hoc explainability technique in the strict sense of the meaning, as attention is contributing to the prediction but typically calculated afterwards to obtain attribute importance scores. These attention layers calculate non-negative weights (multiplied by their corresponding representations) for each input that together sums to one, and finally sums the resulting vectors into a single fixed-length representation [15].

5.3.1 Preprocessing steps
First, an equivalent train-test split as in [2] is performed. To this end, a temporal train-test split is performed that ensures that the period of training data does not overlap with the period of the test data, while the event of the cases in the train data that did overlap with the test data are cut. Next, the traces are cut with similar upper length as defined in [2]. Then, both the index (index) and aggregation (agg) encoding are used to encode the data for the machine learning algorithms. Note that the aggregation encoding is unique to processes, and is the primordial reason to investigate a dedicated OOPPM XAI-based approach. The index encoding is created for traces of all lengths, in contrast to the study of [2], where they used the index encoding for traces with a similar prefix length (i.e. prefix length bucketing technique).

The bidirectional LSTM neural network architecture with attention layers for interpretation purposes stems from [29]. The embedding mechanism is used for categorical attributes in the deep neural networks. Compared to the original set-up, the numerical attributes are added as input layers to the LSTM model. Finally, the predictive function of [29] is transformed into a binary outcome-oriented prediction by stripping off the final layer and inserting a sigmoid output layer instead. In order to compare, ceteris paribus, the overall performance of the LSTM with the CNN, we ensure that both models have a similar set-up. Therefore, the CNN model start from the same architecture as the LSTM, and the Bidirectional LSTMs are replaced with 1D convolutional layers. Different to the LSTM model, the attention is calculated directly after the input layers and embeddings (similar to [50]), and the kernel size is set to be the same as the length of the sequences and the filter as the length of the concatenated input. Additionally, an extra dense layer with Rectified Linear Unit (ReLU) activation was added before the final dense layer, in order to ensure that the output is correctly linked back to the inputs.

The event logs are filtered out for which the average obtained AUC over all the classifiers was lower than 50 (i.e. sepsis cases(2), as no analysis should be performed where random luck has a better ability compared to the classifiers in order to distinguish between the classes). For the XAI evaluation, we additionally filtered out the event logs that had an average AUC below 75 (sepsis cases(3) and production). This was to overcome the issue that explainability techniques can only perform well when the original task model is performant enough.

5.4 Attribute Importance

In case of a black box model, the attribute weights of the task model \( w_{e,1}, ..., w_{e,p} \) need to be measured post-hoc, where for tree-based models a naive method exists in counting the number of times the attributes are selected by the individual trees in the ensemble method [31]. As an improvement, the authors suggest a permutation-based approach by looking at the change in accuracy before and after permuting the attribute values. In this paper, the attribute importance for all black box models are calculated similarly, with the use of a perturbation-based method as described in Algorithm 2 where we evaluate the accuracy change using the Root Mean Squared Error (RMSE). Note that some remarks about this algorithm should be made. First, the attribute importance for the deep learning models is calculated by permuting the original attributes \( \{x'_1, ..., x'_p\} \) instead of the transformed attributes \( \{x_1, ..., x_p\}\). This makes sense for the following reason: the monotonicity value compares the transformed attributes with the original attributes in the explainability model. To ensure that they are both calculated on the same number of attributes, the attribute importance is calculated with the original attributes, and the attention values are aggregated to obtain the importance for the original attributes.

5.5 hyper optimization details

Finally, a 4-fold cross validation was performed with the use of hyperopt for the machine learning models. The hyper
optimization for the deep learning models was done by a 10-fold cross validation, as the neural networks need additional evaluation to overcome the plethora of local minima. For the LR, XGB and RF model, similar hyperparameter settings are taken from [2]. For the LLM model, we additionally incorporate the maximum depth of the decision tree and the minimum samples per leaf to ensure that the tree splitting does not allow overfitting. According to [28], the optimal dropout rate for the bidirectional LSTM with attention was around 0.2. Therefore, we have set the maximal dropout rate to 0.3 (as a margin of error). As a final remark, extra detailed information about design implementations and parameters are provided on GitHub[2] to enhance the reproducibility results.

6 Discussion

As a precursor to the discussion, the predictive performance based on AUC is evaluated in-depth. To have a more profound idea, we use statistical tests to mathematically ground the conclusions. Note that this is separated from the research questions to ensure that the focus remains on the influence of experimental set-up on the introduced metrics.

First, we compare the embedded DL_{embed} models with the ensemble index methods in a similar experimental set-up to Kratsch [3]. For this, we only compare the ML_{index} models with the DL models, as the aggregation encoding is a lossy encoding (see Section 2). The paired t-test ($p_{value} = 0.55$) indicates that the DL_{embed} (87.28 AUC) do not statistically outperform the ensemble index (86.08 AUC), despite having a slightly higher mean. When comparing Table 2 and Table 3, we can see that DL models tend to work best for event logs with a high variant to trace ratio (i.e. the BPIC2015 event logs). We also see that CNNs perform better than LSTMs for logs featuring a high dynamic versus static ratio (BPIC2015(2) and BPIC2015(5)). In addition, many papers state that sequence encoding and extraction of attributes is the most important to increase the predictive performance [3], [4]. Therefore, we expect the index encoding to perform better than the aggregation encoding, as the former provides the predictive model with more information about the sequential development of the process. Contrarily, the paired t-test shows that the ML_{agg} (92.71 AUC) statistically outperforms ($p_{value} = 0.000000003$) the ML_{index} models (85.24 AUC), with the former obtaining the best results in 9 out of 10 event logs. Intuitively, one could argue that the index encoding is potentially underperforming due to an explosion of the attribute space.

In the next subsection, the research questions are answered in-depth. To obtain actionable results, it is required that we link the obtained insights of the research questions with the event log specifications of Table 2. For this, a case-based evaluation in the context of OOPPM is performed with the use of two event logs. This section is finalized with the framework of guidelines for Explainable AI in OOPPM in order to guide the practitioner to the correct model selection. In Table 3, an overview of the AUC results for the encoding-classifier combinations is given.

2. https://github.com/AlexanderPaulStevens/Evaluation-Metrics-and-Guidelines-for-Process-Outcome-Prediction

6.1 Research questions

The first research question RQ1 investigates the influence of the encoding mechanism on the explainability metrics, and Table 1 shows that the use of index encoding over aggregation encoding increases the parsimony $C_F$ and consequently induce more complex explanations. As an example, the parsimony of the event attributes ($C_{event}$) increased with a factor of 15 for the index encoded variant of the $RF_{agg}$ for the event log BPIC2011(2). In a nutshell, the index encoding has generally higher values for parsimony $C_F$ compared to its aggregation variant. Finally, regarding the faithfulness of the model, we observe that the index encoding has a negative impact on the monotonicity $M$ of the explainability model. Moreover, in only two situations, the $M$ was lower for the index encoded variant (sepsis cases (2) and bpic2011(2)). To have a more profound idea, we use statistical tests to mathematically ground the conclusions. Note that this is separated from the research questions to ensure that the focus remains on the influence of experimental set-up on the introduced metrics.

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but the FC of the respective variables are very high, which means that this attribute type was very important for the prediction. This shows that the relative ranking of the FC values is not always similar to the relative ranking of the parsimony CF values. This is considered a problem in cases where the parsimony indicates that a particular attribute type is relatively unimportant, but permutation values these have a very high influence on the predictions (meaning that they are somehow important?). Similar insights can also be obtained from Table 1 (BPIC2015(3)). The GLRM model only uses eight control attributes, but permitting these leads to more than 85% different predicted labels. This answers RQ6.

To answer RQ7, the interpretability-accuracy trade-off does not hold in the field of Outcome-Oriented Predictive Process Monitoring if we look at the average amount of parsimony CF versus the average amount of AUC (results are not reported in the table but can be found on [9]). Conversely, the agg models obtain higher AUC and report lower parsimony CF values. Interesting to see is how well the GLRM model performs with an overall average of 12 attributes (compared to over 625 and 187 for LR and RF respectively), while remaining similarly performant. If we compare the interpretability of the explanations (i.e. defined by the parsimony CF of the control attributes, Ccontrols),

3. https://github.com/AlexanderPaulStevens/Evaluation-Metrics-and-Guidelines-for-Process-Outcome-Prediction
observe a rather high value for $M$ provides insight into the extent to which the performance models perform better than the ML-focused, answering correctly on what attribute types the task model XGB truly that the ranking of the importance of all the attributes was at BPIC2015(3) and the LSTM and CNN model, answering RQ8 $M$ 9/10 event logs for the monotonicity $V_\text{ar.}$ $(\text{index})$ indicates that this event log has a high variant to trace $AUC$ performance. BPIC2011(2), with the latter models reporting the lowest $M$ 6.2 Event log Analysis

A more in-depth analysis is given for two event logs, BPIC2015(3) and BPIC2011(2). In BPIC2015(3), all the $M_{\text{agg}}$ models obtain the best performance, and the DL models perform better than the $M_{\text{index}}$ models. This provides insight into the extent to which the performance is in trade off with the explainability. Contrarily, the $M_{\text{index}}$ models performed better than the DL models in BPIC2011(2), with the latter models reporting the lowest AUC performance.

First, the event log BPIC2015(3) is discussed. Table 2 indicates that this event log has a high variant to trace ($\frac{\text{Var.}}{\text{Trace}}$) ratio (0.96) and high dynamic to static ($\frac{\text{Var.}}{\text{Case}}$) ratio (23.78). These are the event log properties defined by F for which the DL models perform better than the ML models. Next, the LTL rule setting the objective is based on the presence of control flow attributes, which means that we expect a high $FC_{\text{control}}$, which is clearly visible in most of the models. As an example: the $FC_{\text{control}}$ value of the $LLM_{\text{index}}$ for BPIC2015(3) states that more than 98% of the predictions change after permuting the control flow attributes. Furthermore, the $\frac{\text{Case}}{\text{Control}}$ values show that most models still use most of the case (i.e. static) attributes due to the fact that there is a lot of case-specific information in the event logs. In addition, it is also possible to compare the interpretability between different classifiers. Moreover, we see an $FC_{\text{control}}$ of 87.72% for the $XGB_{\text{agg}}$ model, with a parsimony $C_{\text{control}}$ of 74. For the $RF_{\text{agg}}$ model, we observe an $FC_{\text{control}}$ of 81.89%, with a parsimony $C_{\text{control}}$ of 275 control columns. This means that the $XGB_{\text{agg}}$ model uses fewer attributes compared to $RF_{\text{agg}}$, but the attributes used are more important for the predictions made (as 87% percent of the predictions change if these attributes are permuted). From a predictive performance-based perspective, the $RF_{\text{agg}}, LR_{\text{agg}}$ or $LLM_{\text{agg}}$ model is preferred. Nonetheless, the monotonicity $M$ and level of disagreement $LOD\times 10$ values show that the faithfulness of the explainability model of the $RF_{\text{agg}}$ model is compromised. These values indicate that the explainability model is not able to correctly mimic the model behaviour of the task model. This can be due to the fact that the $RF_{\text{agg}}$ model uses all of its attributes (visible with the red colour) based on the values for $C_{\text{control}}, C_{\text{case}}$, and $C_{\text{event}}$. The $LR_{\text{agg}}$ model is faithful by definition, as it generates its own explanations. Nonetheless, the model uses 160 control attributes ($C_{\text{control}}$, but the value for $FC_{\text{control}}$ shows that 1.30% of the predictions change when we permute the control attribute values of the test data (do these 160 attributes really matter for the interpretation of the explanation?). Next, the $LLM_{\text{agg}}$ model obtains the second-best performance, but has a very low value for interpretability (high $C_{\text{control}}$). A next remark is that, although the LSTM model has a considerably smaller attribute space (as the attention values are for the original attributes due to the embedding mechanism), the $M$ appears to be compromised.

Finally, the $GLRM_{\text{agg}}$ uses only eight control attributes ($C_{\text{control}}$), two event ($C_{\text{event}}$) and one case ($C_{\text{case}}$) attribute, while remaining performant (93.79 AUC). The probability of being classified as ‘deviant’ is calculated similarly to a regular logistic regression model [18], with the formula:

$$\log(z) = \frac{1}{(1+e^{-z})}$$

with

$$z=6.35-10.20*(\neg \text{control1}_{\text{agg}} \land \text{control2}_{\text{agg}} \leq 0.5)$$
$$-5.76*(\text{control3}_{\text{agg}} > 0.5) \lor (\text{control2}_{\text{agg}} \leq 0.5)$$
$$-2.86*(\text{control2}_{\text{agg}} \leq 0.5) \land (\neg \text{case1})$$
$$-1.34*(\neg \text{control1}_{\text{agg}} \lor (\text{control2}_{\text{agg}} \leq 0.5) \land (\text{event1} > 7.5))$$
$$-0.97*(\text{control2}_{\text{agg}} \leq 0.5) \land (\text{event1} \geq 7.5))$$

The rules are roughly based on the presence (or absence) of certain control attributes in combination with an event and/or case attribute. To conclude, the use of the GLRM model is advised, as the model is inherently faithful (i.e. creates its own rules) and is highly interpretable while remaining performant in terms of AUC.

Similarly, an analysis for the event log BPIC2011(2) can be made. From a performance-based point of view, the $LR_{\text{agg}}$ is preferred. Nonetheless, it is again noticeable that

![Fig. 3. Interpretability metrics per classifier. The top figure describes the percentage of parsimony $C_{\text{p}}$ of each attribute type individually. The second subplot of Figure 3 shows the percentage parsimony $C_{\text{p}}$ per attribute type, over the total parsimony $C_{\text{p}}$. The bottom subplot shows the $FC_{\text{control}}$ per attribute type.](image-url)
X-MOP: A Guideline to Obtain eXplainable Models for Outcome Prediction

The obtained insights with the use of the research questions and event log analyses are summarized in an XAI-based guidelines map for OOPPM Figure 4. This figure describes the guidelines for Explainable AI purposes in OOPPM. The white boxes are the questions to guide partitioners and researchers in obtaining OOPPM results according to their preferences in terms of predictive accuracy and interpretability. The blue circles are the final recommendations for the sequence encoding and model complexity. Note that the guidelines are designed in a very generic way, e.g., no distinction between the LSTM and CNN based on dynamic vs. static ratio. Nonetheless, we specifically recommend the GLRM model when the interpretability of the model is very important. Finally, the faithfulness metrics only need to be calculated for non-transparent models.

6.3 XMOP: Guidelines for XAI in OOPPM

This paper introduced a framework of metrics to evaluate the explainability of predictive models used for OOPPM purposes. Compared to performance-based metrics, they take into account the event, case, and control perspective and describe the interpretability of the explanations and the faithfulness of the explainability model. Furthermore, we
provide an extensive benchmark study of seven models and thirteen event logs. Finally, we provide the reader with a consistent overview of the insights obtained by this study in the field of OOPPM, and created a framework of guidelines contrasting traditional machine learning, deep learning, preprocessing and explainability approaches to guide the practitioner to the best model selection. Not only can we conclude that the transparent GLRM model exhibits very interpretable explanations for high dimensional and sequential data (for only a small loss of performance), but also that the deep learning models only outperform ML models that are index-encoded. Next, the aggregation encoding is able to improve the explainability-performance trade-off of the index-encoded variant, by obtained a better performing model while offering better interpretability. To conclude, we show that each model has its advantages and disadvantages, where naively opting for the model with the highest performance can have a strong detrimental effect on both the interpretability of explanations and the faithfulness of an explainability model. As a result, identifying faithful explanations, while remaining interpretable, still imposes a challenge for black box models.

One of the limitations of this research is the fact that the metrics do not take the loss of information of the aggregation encoding into account. Therefore, it is assumed that the summary statistics of a certain variable contain no loss in information compared to the original attribute values. Future work will focus on the concept of Responsible AI, by introducing causal inference to assess the causal insights obtainable from predictive models, and focus on the creation of fairness-aware decision models.

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