Local Post-Hoc Explanations for Predictive Process Monitoring in Manufacturing

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Abstract

This study proposes an innovative explainable process prediction solution to facilitate the data-driven decision making for process planning in manufacturing. After integrating the top-floor and shop-floor data obtained from various enterprise information systems especially from Manufacturing Execution Systems, a deep neural network was applied to predict the process outcomes. Since we aim to operationalize the delivered predictive insights by embedding them into decision making processes, it is essential to generate the relevant explanations for domain experts. To this end, two local post-hoc explanation approaches, Shapley Values and Individual Conditional Expectation (ICE) plots are applied which are expected to enhance the decision-making capabilities by enabling experts to examine explanations from different perspectives. After assessing the predictive strength of the adopted deep neural networks with relevant binary classification evaluation measures, a discussion of the generated explanations is provided. Lastly, a brief discussion of ongoing activities in the scope of current emerging application and some aspects of future implementation plan concludes the study.

Introduction

The recent proliferation of internet of things (IoT), cyber-physical systems, cloud computing, enterprise information systems and other smart manufacturing specific technologies, and consequently, the increasing availability of heterogeneous and voluminous production data facilitate the manufacturing firms to establish data-driven intelligence (Lasi et al., 2014). Considered as one of the key enablers of such manufacturing intelligence, artificial intelligence especially machine learning, has been examined throughout the various stages of the manufacturing lifecycle including design, evaluation, operation, maintenance etc. and has already found extensive applications for different problems such as fault detection, predictive maintenance, operations planning, predictive energy consumption monitoring, predictive quality analytics and decision support for various data driven decision making situations (Wang et al., 2018). In their survey based investigation into large corporations, Brynjolfsson et al., (2011) have revealed that adopting data-driven decision-making results in 5-6% increase in their output and productivity. Furthermore embedding data-driven decision-making in business processes yields higher return on investment, return on equity, asset utilization and market value (Provost and Fawcett, 2013).

A growing body of literature has also specifically investigated the added value generated through a successful adoption of one of the key technologies, various enterprise information systems, such as Enterprise Resource Planning (ERP), Customer Relationship Management (CRM), Supply Chain Management (SCM). The empirical findings reveal the necessity and utility of enterprise information systems for facilitating the organizational data-driven decision-making (Hitt et al., 2002). To successfully deploy predictive analytics and establish a data-driven culture in manufacturing firms, a consistent process and information flow as well as their horizontal and vertical integration along the entire value chain have to be ensured. A seamless integration of the top-floor and shop-floor operations and data structures is a decisive point for data-driven intelligence which also constitutes a vital challenge. To address this issue, the Manufacturing Execution Systems (MES) has been established an important enterprise information system that controls, plans and manages the manufacturing operation activities as well as provides an invaluable data source for manufacturing intelligence by capturing highly critical process details including operating data, material data, machine data, planning data, personnel data, energy data, quality data etc.

Process mining has recently emerged as a promising research domain following the objective to generate process specific insights by analyzing the event log data generated by enterprise information systems during the process execution. This study examines a process planning use-case in manufacturing by designing an innovative predictive process analytics and planning solution. To put more precisely, we attempt to develop an explainable process prediction solution by combining process mining and machine learning approaches to enable data-driven decision making by providing relevant explanations for the outcomes delivered by these opaque models. For this purpose, we train first a black-box machine learning approach, deep neural networks, to predict the process outcomes. Following this, two local post-hoc explanation approaches, Shapley values and ICE plots are applied to generate the relevant explanations that facilitate the experts to justify the model decisions.

Related Work

Predictive process analytics referred to as also predictive process monitoring has emerged as a promising branch of process mining aiming at generating predictive insights by using the event log data generated by process-aware information systems (Di Francescomarino et al., 2018) (Evermann et al., 2017). Over time, an extensive literature has developed on predictive process monitoring by focusing on different prediction problems such as next event prediction, business process outcome prediction, remaining time prediction, prediction of activity delays etc. (Breuker et al., 2016; de Leoni et al., 2016; Maggi et al., 2014). However, a thorough analysis of these studies reveals that they mainly use the process data generated from the management level enterprise information systems such ERP, CRM, Workflow Management Systems etc. Only a few studies have examined the predictive process analytics or other branches of process mining such as process discovery, conformance checking or process enhancements in the manufacturing domain by concentrating on the event log data delivered by MES systems (Fettke et al., 2020; Gröger et al., 2012). This study aims to fill this research gap by proposing a relevant process prediction solution.

Furthermore, the literature pertaining to predictive process monitoring suggests that the black-box machine learning approaches provide superior predictive performance compared to traditional comprehensive methods (Mehdiyev et al., 2018). Recently, a considerable amount of research has focused on applying various architectures of deep learning methods (Evermann et al., 2017; Mehdiyev et al., 2018; Tax et al., 2017). Although these approaches deliver more precise prediction outcomes, their lack of explanation constitutes practical challenges for establishing data-driven decision making (Guidotti et al., 2018). Explainable Artificial Intelligence (XAI) has recently reemerged as a research discipline with the purpose to make the communication between artificial advice givers and human users understandable and to establish trust in non-transparent models or their outcomes (Doshi-Velez and Kim, 2017; Gunning, 2017; Miller, 2019). Various studies provide valuable insights into various aspects of XAI research area e.g. by providing an overview of possible taxonomies for explanation techniques (Gilpin et al., 2018; Guidotti et al., 2018; Lipton, 2016), by presenting different mechanisms and approaches for evaluating the explanations (Doshi-Velez and Kim, 2017), by discussing the objectives of XAI solutions (Nunes and Jannach, 2017), by defining the stakeholders of the explanation methods (Preece et al., 2018), by introducing the relevant insights from social sciences (Miller, 2019), by proposing the necessity of considering the findings in cognitive sciences (Fürnkranz et al., 2019) etc. Recently, various studies have been conducted specifically on making predictive process analytics explainable (Mehdiyev and Fettke, 2020a, 2020b; Rehse et al., 2019; Rizzi et al., 2020; Weinzierl et al., 2020).

Methodology and Proposed Approach

To design an explainable process prediction and planning solution, this study follows the Design Science Research (DSR) approach proposed by (Peffers et al., 2007) which combines principles, practices and procedures to conduct applied research. Widely used in information systems research, the adopted DSR comprises six important steps, problem identification, defining objectives of a solution, design and development, demonstration, evaluation and communication of the novelty and rigor to the relevant audience.

Problem Identification

A thorough incorporation of various process-aware enterprise information systems over various stages of the production automation pyramid enables to carry out different process specific analytics. A robust and reliable process planning solution should support the domain experts in defining the sequence of operations and processes, identifying the resources, conducting time, cost and risk specific estimations and finally in defining preventive measures by proactively monitoring the deviations from the desired outcomes. Predictive process analytics offers enormous possibilities to realize the concept of data-driven process planning in manufacturing. However, most of successful process prediction approaches are mainly black box approaches and due to their non-transparent nature, they fail to deliver the relevant explanations about their outcomes or inferencing process. This in turn reduces the trust in models and introduces the acceptance barriers in using data-driven process specific solutions even though they often deliver more superior outcomes compared to judgmental and intuition-based decisions.

Objective of a Solution

The objective of the proposed solution is embedding the data-driven decision making into the predictive process planning and analytics. To generate a trustworthy, consistent, and sufficient predictive process planning solution for a manufacturing firm, in the first step it is essential to ensure that high quality data from relevant enterprise information systems are acquired, integrated, appropriate feature pre-processing and extraction approaches are thoroughly carried out and finally sound machine learning models with strong predictive power are constructed and consequently validated.

Another preliminary and ultimate objective of the proposed solution is the operationalization of the recommendations and insights delivered by adopted advanced machine learning models for process predictions by making them explainable and interpretable. Generating explanations for black-box machine learning approaches pose complex challenges since various properties of the decision-making environment, the requirements of the target audience and other economic, organizational, and legal considerations influence the appropriateness of explanations significantly. Therefore, to conduct the explanation generation process systematically, we follow the conceptual framework proposed by Mehdiyev and Fettke (2020b) which was designed to guide the developing explainable process predictions solutions. According to this framework it is crucial to identify the target audience of the explanations, to define their objectives, to examine the context of explanation situation and to choose the adequate techniques that can facilitate the users to attain their goals.

In this study, the domain experts who have deep expertise in process and production planning but with little machine learning background are defined as the main target audience. These users prefer to justify the outcomes delivered by machine learning models rather than to understand the complicated inner working mechanism of these opaque models. Such a ratification goal of the model recommendations enables the experts to verify whether the model findings conform to their knowledge and expertise, to learn the complex relationships especially in weak theory domains and to identify the preventive measures. To this end, it is conceivable to suggest that post-hoc explanation tools are the most appropriate tools which attempt to open the black-box models once the models are already trained. Since the domain experts in our case are more interested to understand every single model decision, we propose to adopt the local post-hoc explanation approaches.

Design and Development

This section provides an overview of the steps carried out to develop an explainable process analytics and planning solution. In the proposed approach, the machine learning features have to be extracted once the data from various enterprise information systems are aggregated, cleaned, and harmonized. Particularly, MES-driven process-specific features such as total number of process steps required to produce the planned manufacturing part, average duration per process step, average energy consumption per process step, planned setup time, Overall Equipment Effectiveness (OEE), employee effectiveness etc. are used as input variables for the black-box machine learning approach to predict whether the quality of the produced parts fulfill the pre-defined requirements or not. To address this binary classification problem, this study deploys a deep feedforward neural network. Table 1 provides an overview over the parameters of the adopted deep learning approach.

Parameter	**Value**
Initial Weight Distribution	Uniform Adaptive
Activation Function	Rectifier with Dropout
Input Dropout Ratio	0.2
Hidden Layer Dropout Ratio	0.5,0.5,0.5,0.5
Epochs	1000
Adaptive Learning Rate Algorithm	ADADELTA
Rho (adaptive learning rate time decay factor)	0.99
Epsilon (adaptive learning rate time smoothing factor)	1e-8
Max w2 (the constraint for the squared sum of the incoming weights per unit)	100
Early Stopping Metric	AUROC
Stopping Rounds	5
Stopping Tolerance	0.005

Table 1. The Parameters of Deep Feedforward Neural Networks

After having verified and validated the predictive performance of adopted deep learning, two local post-hoc explanation approaches, Shapley Values, and Individual Conditional Expectation (ICE) plots are used to explain every single outcome of the model. As one of the widely recognized feature-attribution based explanation technique, the goal of Shapley explanations is adapting the cooperative game theory to machine learning interpretation. In this context, the values of the input features for the examined instance are treated as game players and the classification model prediction scores as the corresponding payoffs. To complement the Shapley value-based explanations, this study also generates ICE plots which are expected to allow the users to check how the model reacts to the changes in the values of the plot variable for the examined observation. A combination of these two local post-hoc explanation techniques is presumed to provide a more comprehensive explanation for justifying the model outcomes.

Demonstration, Evaluation and Communication

To demonstrate the applicability of the proposed explainable process prediction solution, we investigate the process planning use case in a medium sized manufacturing firm operating in the field of tool and fixture construction. Due to the limited availability of real production data at this stage of the research project, we use semi-artificially generated data partially based on the initial input delivered by the implemented MES system at the partner manufacturing firm and feedback from process experts to achieve as close as possible data structures reflecting the real situation of examined processes. We adopted the data generation approach based on radial basis function networks proposed Robnik-Šikonja (2015) which learns sets of the Gaussian kernels and uses them to generate data from the same distributions.

Performance of the Black-box Model

To assess the predictive strength of the adopted deep neural networks, we compute and introduce threshold-free evaluation measures such as area under ROC Curve (AUROC), area under Precision-Recall Curve (AUPRC) and various single-threshold measures. The obtained AUROC and AUPRC are illustrated in the Figures 1 and 2, respectively.

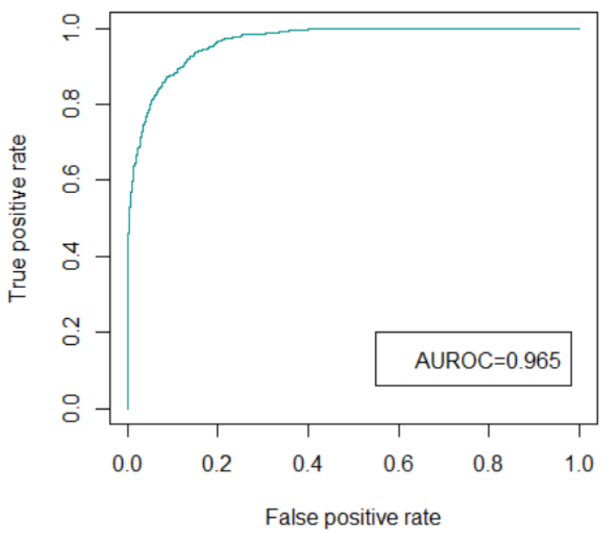

Figure 1. Area under ROC Curve Obtained by the Deep Neural Network

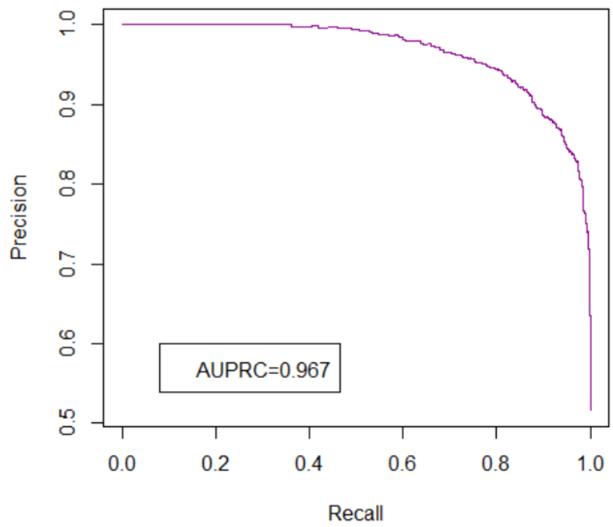

Figure 2. Area under Precision-Recall Curve Obtained by Deep Neural Network

For single-threshold binary classification evaluation measures, the cut-off threshold is defined at which the Matthews correlation coefficient (MCC) is maximized. Table 2 presents the obtained binary classification evaluation measures at the defined cut-off threshold of 0.409.

Evaluation Measure	**Value**
F1-Measure	0.901
F0.5-Measure	0.881
Accuracy	0.894
Precision	0.869
Recall	0.9357
Specificity	0.849
Absolute Matthews correlation coefficient (MCC)	0.789
False Negative Rate	0.064
False Positive Rate	0.150

Table 2. Binary Classification Evaluation Measures

As has been previously suggested in the literature on explanation for intelligent systems an inaccurate explanation can be misleading and is worse than no explanation at all (Swartout and Moore, 1993). In this context, (Zhao and Hastie, 2019) suggest that the first prerequisite for successful explanations is the good predictive model. The AUROC (0.965) and AUPRC (0.967) values as well as various single-threshold measures of interest particularly the absolute MCC (0.789) and F1-Measure (0.901) suggest that the applied machine learning technique achieves strong predictive performance that fulfill the pre-defined success criteria.

Local Post-Hoc Explanation with Shapley Values and Individual Conditional Expectation Plots

After verifying and validating the performance of the adopted neural networks, we can now generate the relevant local post-hoc explanations for process domain experts and production planners. This subsection introduces Shapley values and ICE plots for randomly chosen observations with true negative (Failed) and true positive (Passed) predictions. Furthermore, a discussion on harmonic transitions between chosen both local post-hoc explanation approaches is provided which are presumed to enhance the decision-making capabilities of experts by enabling them to examine the explainable process predictions from different perspectives.

Figure 3 introduces the Shapley values for an observation with a true negative prediction. The respective Shapley value suggests that the Overall Equipment Effectiveness (OEE) of 0.44 in the examined instance decreases the probability for the class "Passed" significantly. The observed value of another MES specific KPI, the employee productivity, pushes the probabilities towards a negative direction as well by increasing the probability for class "Failed". Although all other variables increase the probability in favor of positive class, their contribution are too small to change the model's decisions.

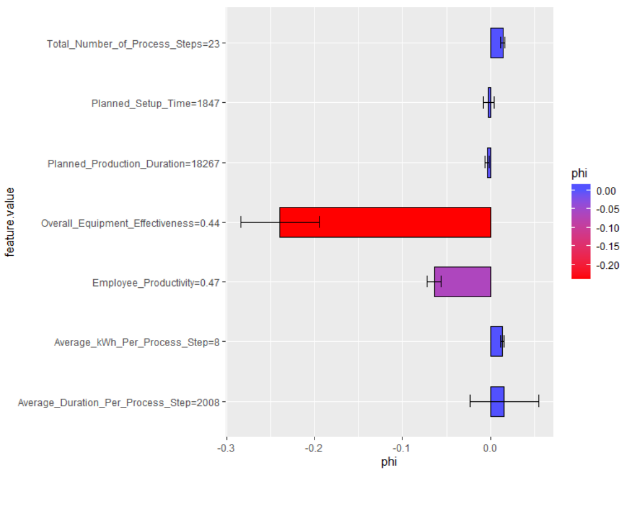

Figure 3. Shapley Values for the Observation with True Negative Prediction

Figure 4 introduces the Shapley values obtained for the observation which was correctly predicted as "Passed" with the prediction score of 0.86. According to the obtained Shapley values, the higher value of OEE in this case is strongly associated with high prediction score in favor of class "Passed". Furthermore, the higher value of employee productivity has also a positive impact on the prediction scores. A thorough examination of other features contributions suggests that even though in this observation more features have negative Shapley values compared to the previous instance, the impact of the most influential two features lead to an overall increase in the prediction score of the positive class.

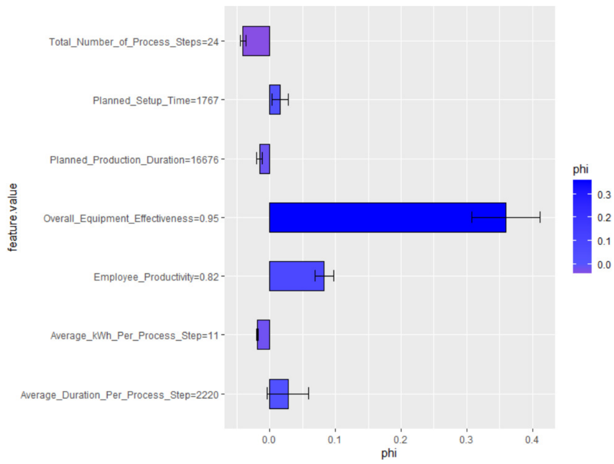

Figure 4. Shapley Values for the Observation with the True Positive Prediction

The Shapley values provide very useful information on contribution of each feature value to the model outcome; however, it has a static nature which provides only the snapshot of the situation by examining the given fixed feature values. By introducing the ICE plots, we can generate complementary explanations that allow to examine how the predictions of each observation change when the feature values change. The main working principle of ICE plots is intuitive. For the examined instance, we choose every time a plot variable of interest and generate new instances by changing its value by the using the values from the pre-defined grid and keeping the values of all other variables' constant. The generated instances are then fed to the underlying black-box model and obtained prediction scores over different values of the plot feature are visualized. For illustrative purposes, the ICE curves for chosen plot variables, OEE, employee productivity and average duration per process step are presented.

Figure 5 suggests that in both cases an increase in the OEE values has positive impact on prediction scores (Passed). This aligns with the Shapley based explanation introduced above. The green ICE Curve which represents the observation with true positive prediction implies that the OEE value of 0.95 results in very high prediction score. This feature is so important for this observation that that an important decrease in its values may decrease the probabilities and lead to a negative outcome. At the same time, the analysis of the ICE Curve for the observation with true negative prediction (presented with red line) suggests that a considerable increase in its current value (0.44) may switch the model decision to positive outcome.

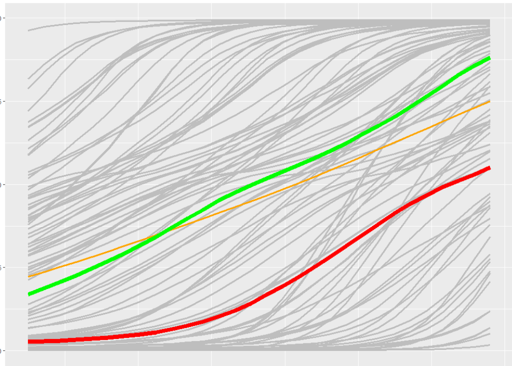

Figure 5. ICE Plots for Overall Equipment Effectiveness

As depicted in the Figure 6, the similar trend can be observed in both ICE plots for the employee production feature. An increase in the values of these variables increases the prediction probability of being classified as “Passed”, positive class. This interpretation can also be easily linked to the Shapley explanations. The feature value in the case of observation with true negative prediction (0.47) is considerably lower than the value for the observation in another examined instance (0.82). Therefore, in the first case it has negative Shapley values whereas the Shapley value in the second case push the probabilities in favor of positive class.

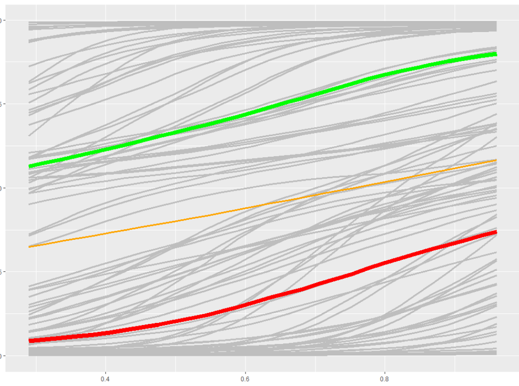

Figure 6. ICE Plots for Employee Productivity

Finally, the Figure 7 presents the ICE plots for the average duration per process step. The both ICE plots (red and green lines) follow the similar trend. In contrast to the ICE plots for two previously examined features, an increase in the average duration per process step decreases the prediction scores for good quality. The values for this feature are close for both observations (2220 vs. 2000 seconds) and are positioned in a critical point because an increase after around 2000 seconds results in sharper decrease of the prediction scores for class “Passed”. By using the explanations generated by these ICE plots, the domain experts can adapt the process plans by defining relevant strategic measures for reducing the average duration per process step which may lead to the outcome with higher qualities.

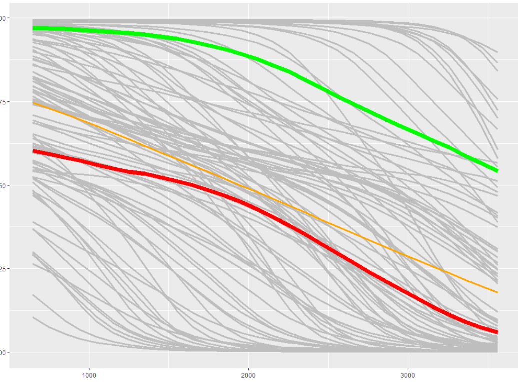

Figure 7. ICE Plots for Average Duration per Process Step

Discussion and Conclusion

The main objective of this study was proposing an explainable process prediction solution to facilitate the data-driven decision making for process planning in manufacturing. After a thorough data preparation phase, a deep neural networks approach was applied to predict the process outcomes in terms of the defined quality criteria. After defining the domain experts as the main target audience and their justification purpose of the model outcomes, we generated the relevant explanation by using two complementary local post-hoc explanation approaches, Shapley values and ICE plots. It is worth mentioning that in the scope of the underlying research project, we also examine the applicability of various local post-hoc explanation approaches such as LIME, counterfactual explanations, case-based explanations etc. Furthermore, our future research work also pursues the objective of developing novel local post-hoc explanation approaches to overcome various shortcoming of perturbation-based techniques. Moreover, future research could examine various global post-hoc explanation techniques and investigate their harmonic combination with local explanation techniques. It is worth mentioning that this study introduces the preliminary results of an ongoing research project. The next stages of the implementation plan include generating explainable process predictions with real process data, identification of the technical requirements for deployment in the production facilities and performing the usability evaluation by using explanation evaluation procedures and methods in terms of various desiderata.

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