

ExMed: An AI Tool for Experimenting Explainable AI Techniques on Medical Data Analytics

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Abstract—The recent explosion of demand for Explainable AI (XAI) techniques has encouraged the development of various algorithms such as the Local Interpretable Model-Agnostic Explanations (LIME) and the SHapley Additive exPlanations ones (SHAP). Although these algorithms have been widely discussed by the AI community, their applications to wider domains are rare, potentially due to the lack of easy-to-use tools built around these methods. In this paper, we present ExMed, a tool that enables XAI data analytics for domain experts without requiring explicit programming skills. In particular, it supports data analytics with multiple feature attribution algorithms for explaining machine learning classifications and regressions. We illustrate its domain of applications on two real world medical case studies, with the first one analysing COVID-19 control measure effectiveness and the second one estimating lung cancer patient life expectancy from the artificial Simulacrum health dataset. We conclude that ExMed can provide researchers and domain experts with a tool that both concatenates flexibility and transferability of medical sub-domains and reveal deep insights from data.

Index Terms—Explainable AI, Medical Data Analytics, Explainability, Interpretability, COVID-19, Cancer.

I. INTRODUCTION

Explainable AI (XAI) has drawn tremendous attention in the recent years [1]. XAI systems not only aim to make intelligent decisions or accurate predictions, but also provide an insight into the process of AI decision making [2]. A goal of enabling explainability in AI systems “is to ensure algorithmic predictions and any input data triggering those predictions can be explained” [3]. In the context of Machine Learning (ML), XAI focuses on developing human-understandable prediction models producing explanations, along with predictions and model agnostic techniques that generate explanations to existing ML models.

From a data science perspective, equipped with its “explanation power”, XAI is not only useful in bringing trust to AI models [1], but is also about providing deeper insights from data. By explaining why an AI model makes a certain prediction, one also gains knowledge about the underlying data used to build the model. As a relatively new field, current development in XAI software is fragmented and implementations are scattered in multiple libraries written in

different programming languages, predominately intended for data science developers rather than domain experts. The lack of easy-to-use XAI tools also hinders further development of XAI.

In this paper, we present ExMed, a self-contained XAI toolkit for domain experts that performs XAI analysis for prediction models. With its simple user interface, it supports both *global* explanations presenting patterns of the entire dataset and *instance* explanations that are local to individual predictions, for both classification and regression tasks. Although various XAI techniques have been proposed in recent years – e.g., a good overview of these techniques is presented in [4] – we focus on feature attribution explanation techniques [5] due to the transparency of their explanations, their computational effectiveness and general popularity.

We also present two real world case studies that demonstrate ExMed’s functionalities. In case study I, a COVID-19 transmission study reveals how different COVID-19 control measures were used and impacted transmission rates. In case study II, we examine lung cancer patient life expectancy using the Simulacrum dataset.¹ Through the two case studies, we illustrate how ExMed can be used for making predictions and generating explanations.

II. RELATED WORK

The use of Machine Learning (ML) has become more prominent in several areas of healthcare, such as diabetes, arthritis, cancer [6]–[8], with varying input formats ranging from tabular data in stored in relational databases to large scale image datasets [9]. Stemming from the involvement of data sensitivity in the medical domain is the necessity of gaining human trust towards ML application [10]. Thus, we see a recent surge in the production of interpretable results using state-of-the-art models such as Local Interpretable Model-Agnostic (LIME) [11] and SHapley Additive exPlanations (SHAP) [5] to supplement the outputs provided by black-box algorithms, with much work showing the intent of XAI expansion through new prediction model architectures [12], [13].

XAI aims to improve the usability of AI by providing justifications behind a given ML prediction [14]. It is a field of exploration by creating a framework to cater for usability

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¹<https://simulacrum.healthdatainsight.org.uk/>

adhering to each step of an ML pipeline, including data manipulation, pre-processing methods and explainability. Whilst yielding the same prediction performance, the explainable aspect helps reduce bias and promote fairness of the prediction model. This interpretable aspect in junction with human input can then create an optimal pipeline of fairness whilst obtaining best results by providing reasons and insight to a decision making process.

Currently, many ML pipelines are especially designed for identifying a problem with a high degree of specificity and pipelines often need to be reconstructed with new data. Without basic knowledge of ML, accessibility to ML applications can be limited without support of ML domain experts. In addition, there is a demand for more human-input and interaction within the AI model to support explainability [15], [16], with the exploration of explainable architectures having received recently some important development from web-based interfaces supporting image segmentation with a readily available interface [17].

A few open-source applications have been developed to ease the application of AI to various datasets, e.g., [18]–[21]. Since so much data in biology is saved as images and Fiji [18] is an example of an open-source tool designed exclusively for biological-image analyses that aims to prototype algorithms for image-processing.

MOA [20] is platform to use for data stream and applications that needs prediction be done quickly. Data arrives in a stream of instances. Each instance can be used as test before using it as train instance. Showing outliers and clustering datas are a part of feature in MOA. Both Fij and MOA are not close to the kind of dataset that we focused on.

WEKA [19] is another workbench designed to combine different ML libraries for supporting various analysis through a graphic user interface. WEKA creates fast access to the information within the datasets, allowing selection of areas of interest. In this platforms can do some data-preparation such as casting, replacing and numeric transform , and also applying machine learning algorithms e.g regression,classification,regression. WEKA, however does not provide both merging and concatenation of datasets, which is often required when introducing new medical data.

We’ve included useful data preparations for the majority of medical datasets in nutshell. Another feature that is not found in other softwares is explanantions. Visualization is also an important aspect of our software.

III. EXMED WORKFLOW

When sending medical data to an ML model, human errors and noise can reduce the quality of the results. Moreover, as one of the leading challenges in medical data analysis is to aggregate data from multiple data sources for performing joint analysis [22], it is crucial for medical data analytic platforms to support the pre-processing stage. Our new application ExMed [23] addresses both challenges and makes the integration of data pre-processing tools easier in order to minimise error and increase the baseline performance of the ML model.

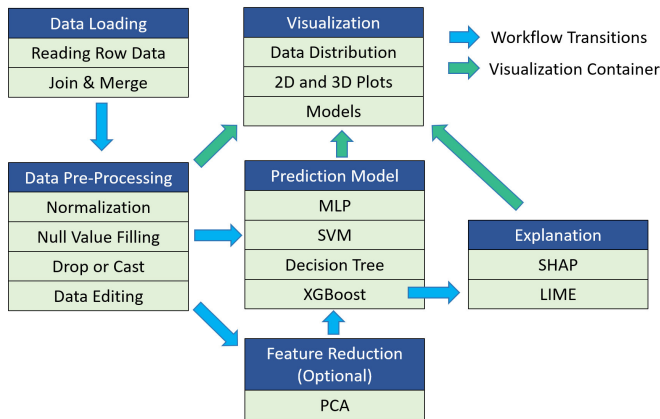


Fig. 1: ExMed Activities. ExMed provides the user with a sequence of simple actions, including loading, merging and editing data, and creating prediction as well as explanation models. Various visualisation techniques are supported in several stages of this pipeline.

ExMed’s main functionalities and architecture illustrations are shown in Figure 1 and 2. ExMed implements a wide set of tools to load, process, predict, interpret and explain data. Its back end design is modular so that more tools can be easily added at a later stage. ExMed can accept most common data files as input (e.g. Excel, CSV, or SAS, and XPT files) with the possibility for easy integration of new file types. Input data can be then combined through classic database join operators, whether or not a common key exists. This gives users the potential to create larger datasets from different file types – potentially collected from different sources – rapidly. Cells, rows, columns and data types can be edited by the user directly within ExMed, allowing greater freedom for data manipulation and quality checks. Data validation is supported by various visualisation tools included with the interface. These tools can represent data trends in many ways (see Fig ?? for a few examples) to provide fast data insight to users and can be applied to either the entire dataset or just part of it.

Creating a model can easily be done by selecting a target label (i.e., column) in the interface. Non-categorical columns selected from inference can be edited and transformed into a category (e.g., using a thresholding operator, Fig. ??) prior to creating the model. Once data has been finalised and validated, and a target label has been created, a range of machine models can then be applied, including SVM, Random Forest Classifier, MLP Regression and XGBoost. There is also an option to apply dimensionality reduction by preprocessing data with an automated Principal Component Analysis (PCA) process. Moreover, the result of the PCA can be visualised in 2D or 3D from the two or three largest eigen vectors respectively.

To interpret data, individual models have their own functions to offer specific explanations. SHAP dot plots, SHAP bar plots, SHAP dependence plots and LIME plots can be used for this purpose. This will show different ways of explaining the reasoning behind the results. We explore explanations and ExMed capabilities on two case studies in sections IV and V. LIME and SHAP adhere to ML local interpretability requirements

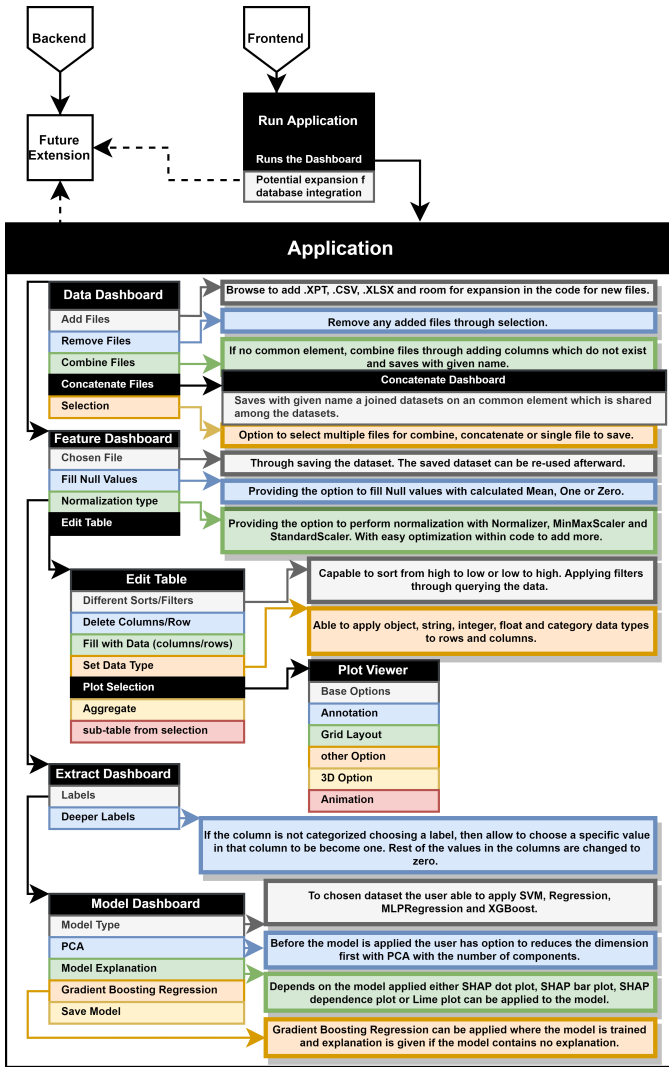


Fig. 2: ExMed Operation Overview. This figure shows the flow of ExMed operations, along with the key features available in the interface. Once the "Application" is running, the first window "Data Dashboard" is shown. Black arrows denote event-driven actions that take the user to the next window in chronological order. Colours highlight the Key features for each window, along with a short description provided for each feature. The indentation of boxes represents a dependency between windows. For instance, the 'Feature Dashboard' window can lead to the 'Edit Table' window, which subsequently can open the 'Plot Viewer' window. The dotted line represents a database extension that is to be added in the future.

for patient instances; expressed as a necessity from clinicians [10], whilst also producing global explanations. To invoke trust, we provide explanations from both LIME and SHAP as both models see a lack of ubiquity in feature priority, but may still provide valuable insight into the data as these methods still often see the same trend in feature attribution [24]. Also, feature attribution algorithms allow for a better understanding of data, as we are able to visualise bias, error, and gain insight into patient instances.

TABLE I: Non-pharmaceutical COVID Control Measures.

Control Measures	Type
Meeting Friends / Family (Indoor)	Categorical
Meeting Friends / Family (Outdoor)	Categorical
Domestic Travel Control	Categorical
International Travel Control	Categorical
Cafes and Restaurants Control	Categorical
Pubs and Bars Control	Categorical
Sports and Leisure Closure	Categorical
Hospitals / Care and Nursing Home Visits	Categorical
Non-Essential Shops Closure	Binary
School Closure	Binary

IV. CASE STUDY I: COVID-19 CONTROL MEASURES

In this case study, we demonstrate how ExMed can be used in investigating relative effectiveness of COVID control measures used in the UK.

From the Public Health England website², we collect daily infection numbers reported across 9 regions in England *East Midlands, East of England, London, North East, North West, South East, South West, West Midlands, and Yorkshire and the Humber*, as well as and the other three nations in the UK: *Wales, Scotland and Northern Ireland*. Non-pharmaceutical control measure data were collected based on UK's COVID policies as summarised in Table I. Data are collected from from various sources including the Wikipedia and major news agencies such as BBC. Control Measures are coded based on the level of severity ("High", "Moderate" or "Low") for all control measures excluding Non-essential shops and School closures, which are coded as binary choices ("Open" and "Closed"). Temperature and humidity data obtained from the weather website Raspisaniye Pogodi Ltd³ were also included. This represents a total of 4,257 data points that were collected between February 2020 and February 2021.

We study the effectiveness of control measures by observing their impacts to the virus transmission rate R_t . Specifically, from daily infection numbers, we estimate R_t using the method reported in [25], [26]. R_t is one of the most important quantities used to measure the epidemic spread. If $R_t > 1$, then the epidemic is expanding at time t , whereas if $R_t < 1$, then it is shrinking at time t . A *serial interval distribution*, which is a Gamma distribution $g(\tau)$ with mean 7 and standard deviation 4.5, is used to model the time between a person getting infected and he/she subsequently infecting another person on day τ . The number of new infections c_t on a day t is computed as:

$$c_t = R_t \sum_{\tau=0}^{t-1} c_\tau g_{t-\tau}, \quad (1)$$

where c_τ is the number of new infections on day τ ,

$$g_1 = \int_{\tau=0}^{1.5} g(\tau) d\tau,$$

and for $s = 2, 3, \dots$,

²<https://www.gov.uk/government/organisations/public-health-england>

³https://rp5.ru/Weather_in_the_world

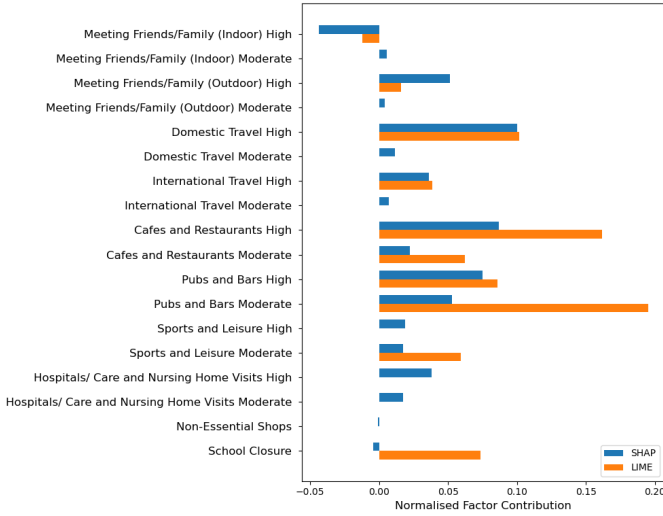


Fig. 3: Example of an Explanation computed with SHAP and LIME. For this instance, both explainers consider top measures contributing to this prediction being *Domestic Travel*, *Cafes and Restaurants Closure* and *Pubs and Bars Closure*.

$$g_s = \int_{\tau=s-0.5}^{s+0.5} g(\tau) d\tau.$$

From Equation 1, we have:

$$R_t = \frac{c_t}{\sum_{\tau=0}^{t-1} c_\tau g_{t-\tau}} \quad (2)$$

For $x = t$ and τ , c_x is the difference between the confirmed case on day x and the confirmed case on day $x - 1$, which is available from the dataset directly.

Using this data, we pose a simple classification question:

Given the infection number and control measures implemented on a day t , can we predict $R_t \geq 1$?

As control measures take time to affect the infection rate, we expand the dataset to include the duration of control measure implementation for all control measures. For example, “*Meeting Indoors (High) = 2*” means that “*it is the second week that meeting indoors has been banned completely*”. Similarly, “*International Travel (Low) = 0*” means that “*there is no restriction implemented on international travel*”. We also drop instances before March 15, 2020 across all 12 regions and nations in our dataset due to the low number of infections.⁴ In this way, we form a data file with 18 features and 3,937 instances with 1,550 positive ones.

TABLE II: Prediction performance on the COVID dataset with four different classifiers.

Classifier	MLP	Random Forest	SVM	XGBoost
Precision	0.87	0.90	0.87	0.87
Recall	0.79	0.84	0.78	0.79
F1-score	0.83	0.87	0.83	0.84

The classification results are summarised in Table V. We can see that all four classifiers are able to achieve good

⁴As can be seen from Equation 2, when c_x is small, R_t can flatten in a unrealistically large range and generate noises in the dataset.



Fig. 4: Global explanations generated using SHAP on our COVID dataset for the prediction whether $R_t \geq 1$. We see that closing down cafes and restaurants as well as pubs and bars are the most effective control measures. When their feature values are high (red), they have string negative impact to the prediction; whereas when their feature values are low (blue), they have strong positive impact to the prediction.

performance on this dataset with a 70/30 training/testing split. As an illustration, for a prediction query instance such that:

- all control measures shown in Table I except *International Travel (IT)* and *Hospital / Care and Nursing Home Visits (HCNHV)* are implemented for more than 35 days at the level *High*;
- *IT* has been implemented for more than 35 days at the level *Moderate*; and
- *HCNHV* implemented for 20-25 days at the level *High*.

Using Random Forest as our prediction model, it correctly predicts that $R_t < 1$; and SHAP and LIME explanations are shown in Figure 3. We see that SHAP and LIME produce similar explanations for the instance. In addition to local explanations, ExMed can also use SHAP to compute global explanations for the entire dataset - describing the “trend” of all instances - as illustrated in Figure 4. We observe that control measures *Cafes and Restaurants Control* and *Pubs and Bars Control* have the most influence to predictions made with this dataset, this can be interpreted as:

From February 2020 to February 2021, the most effective non-pharmaceutical COVID control measures implemented in the UK are closing cafes and restaurants as well as pubs and bars.

V. CASE STUDY II: LUNG CANCER LIFE EXPECTANCY

Our second case study investigates the application of XAI to electronic patient records for cancer research instead of using public health epidemiology data in order to emphasise the transferability provided by ExMed. Especially, we use artificial data from the Simulacrum⁵, a synthetic dataset devel-

⁵<https://simulacrum.healthdatainsight.org.uk/>

TABLE III: Each patient is described with 20 features.

Feature	Value	Feature	Value
ACE	2.0	T Best	0.0
Sex	M	M Best	3.0
CNS	9.0	N Best	4.0
Age	68	Cycle Number	0.0
Grade	0.0	Ethnicity	1.0
Height	1.6	Cancer Plan	1.0
Weight	75.6	CReg Code	4.0
Morph	8041.0	Chemo Radiation	N
Laterality	901.0	Regimen Time Delay	N
Performance	1.0	Regimen Stopped Early	N

oped by Health Data Insight CiC and derived from anonymous cancer data provided by the National Cancer Registration and Analysis Service⁶, which is part of Public Health England. This dataset contains 1,322,100 cancer patient instances.

We first isolate a cohort of interest, opting for lung cancer patients as they represent a large portion of cancer-based deaths [27]. With lung cancer patients, we define the medical question as a prediction of patient survival time, and pose the following multi-class classification question:

Given a set of features for a patient, what will be the predicted survival time for the patient? Under six months, six to twelve months, or more than twelve months?

To study this, we first identify the subset of lung cancer patients in the Simulacrum with an ICD-10 code “C34” *Malignant neoplasm of bronchus and lung* and a deceased status, and includes 108,282 patients in total. We removed records from the original dataset with obvious errors and included only patients with a vital status date posterior to the diagnosis date.

A major challenge in medical data analytic, as exemplified in the Simulacrum, is missing or incomplete patient records. This results in a large number of “null” entries in the dataset. To address this, we identify a smaller cohort of patients such that each patient contains 20 features, with each patient instance only able to contain a maximum of one “null” value. This explicit filtering isolates a cohort of 2,260 patients. This also provides a well-balanced dataset with each group containing a similar amount of patients as shown in Table IV.

TABLE IV: Survival Time Feature Value Count

Survival Time	Value Count
<i>Greater than 1 Year</i>	842
<i>Between 6 Months and 1 Year</i>	748
<i>Less than 6 Months</i>	670

TABLE V: Prediction performance on the Lung Cancer dataset with four different classifiers.

Classifier	MLP	Random Forest	SVM	XGBoost
Precision	0.86	0.90	0.77	0.69
Recall	0.76	0.90	0.98	0.66
F1-score	0.81	0.90	0.86	0.67

⁶<http://www.ncin.org.uk/>

We first provide a local explanation example using both SHAP and LIME for a patient instance as shown in Table III. We observe that both explainers give similar explanations as shown in Fig 5. Using the entire dataset, we produce a global explanation determining feature importance towards each output class in Fig 6 (a). We then provide granularity to feature value importance towards each class with Fig 6 (b) - (d). We interpret these results as:

Cancer grades, BMI, age, patient performance and the absence of distant metastatic spread are key indicators for estimating patients survival time.

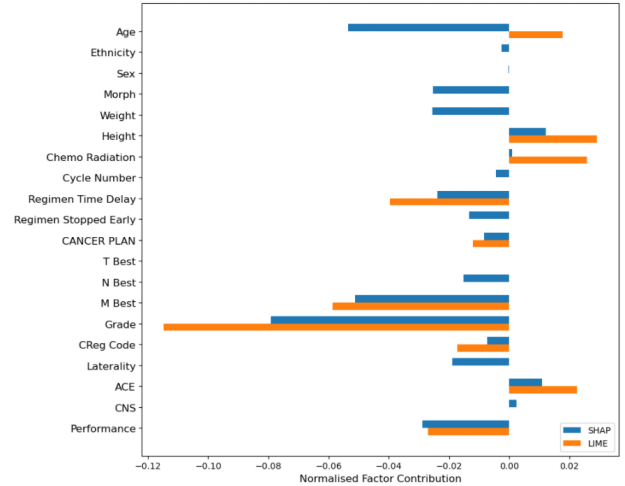
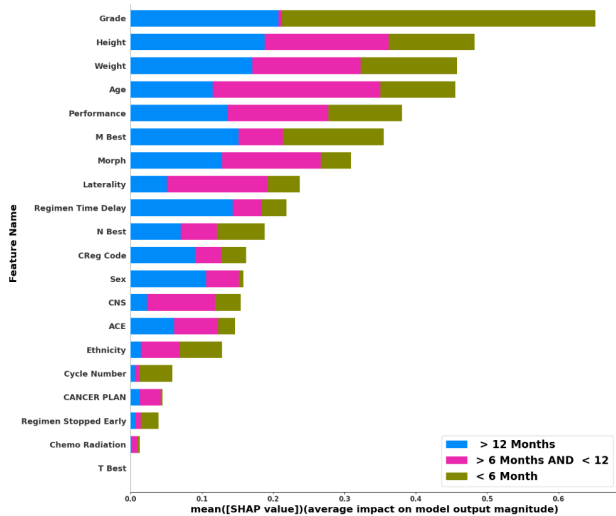


Fig. 5: Local explanation on the Lung Cancer life expectancy data set for a patient instance. We see that the most impactful features amongst SHAP and LIME are the same: “Grade” *How the cancer cells act; the higher the grade the less normality the cell resembles and it may act more aggressive* and “M Best” *Presence or Absence of Distant Metastatic Spread*, followed by a disagreement on age attribution.

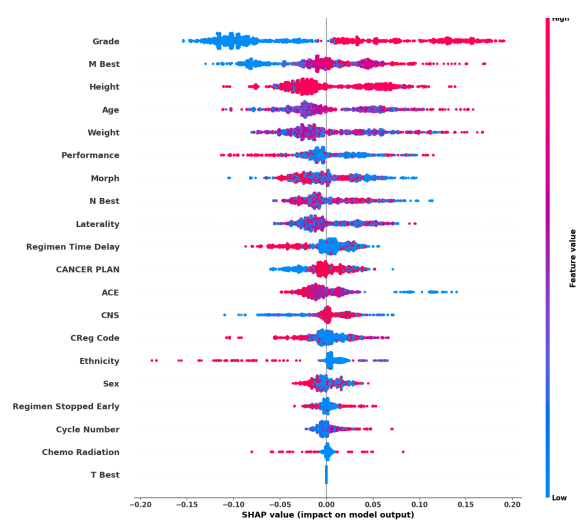
VI. CONCLUSION

In this paper, we present ExMed, a self-contained software package that enables Explainable AI data analysis for medical domain experts without the need for explicit programming. With the development of ExMed, we aim to provide a tool that both concatenates the flexibility of medical sub-domain transferability and obtain an essence of trust through explainability using XAI methods. ExMed accepts multiple data input types and supports several standard pre-processing operations. It employs a number of different prediction models and visualisation techniques, while implementing two popular feature attribution XAI algorithms.

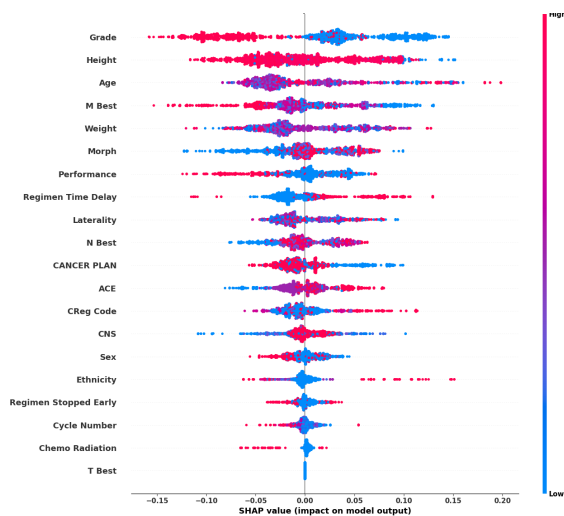
We have experimented ExMed with two real-world case studies in the domains of epidemiology in public health and cancer research with electronic patient records. In particular, we have studied effectiveness of COVID control measures in the UK using data from March 2020 to January 2021 and the life expectancy of lung cancer patients using the Simulacrum dataset. From the COVID case study, we observed that closing



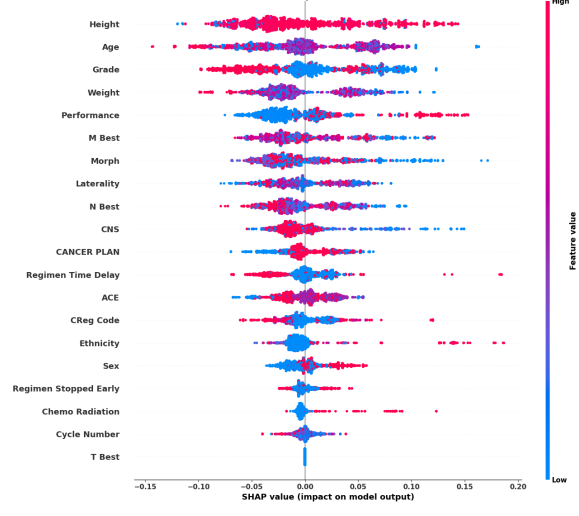
(a) We see that the largest impact towards the survival boundaries *greater than 1 year and less than 6 months* is the cancer grading - having direct impact on the longest and least time survived. This, followed by an associative relationship between height, weight and the patient age determinants of body mass index (BMI), having high attribution towards each class. This, then followed by cancer specific traits such as “M Best” and laterality of the tumour.



(b) Global explanation for feature attribution measured against the class *Survival time of less than 6 months*, where we see the cancer grade of higher value - indicative of cell abnormality and more aggressive, followed by “M Best” *Presence or Absence of Distant Metastatic Spread*, with the associative BMI attributes “height”, “age” and “weight” following this.



(c) Global explanation for feature attribution measured against the class *Survival time of greater than 12 months*, we see an inverse plot of cancer grade to that shown in Fig.6 (a), such that a lower grade and what seems to be a better controlled BMI and a lower “M Best” contributing to a longer survival time.



(d) Global explanation for feature attribution measured against the class *Survival time between 6 and 12 months*, we see that a controlled BMI and lower cancer grade are attributive to this survival boundary, whilst the distributive “M Best”, performance and cancer grade containing high values in both positive and negative impacts on the model are likely the reason for the central survival boundary.

Fig. 6: Global explanations on the lung cancer life expectancy data set.

down cafes and restaurants as well as pubs and bars had the most impact in reducing the virus transmission rate. From the cancer case study, we saw that cancer grades, BMI, age and M Best are amongst the most influential factors for survival.

In the future, we plan to (1) experiment ExMed with healthcare professionals and conduct user studies to evaluate effectiveness of various XAI approaches; (2) further expand the functionality of ExMed and explore features such as parameter tuning; (3) incorporating additional missing value

imputation techniques such as MICE [28] and SICE [29]; and (4) introducing additional XAI techniques such as Anchors [30] in ExMed.

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