Research Internship (PRe)

Field of Study : Explainable AI
Scholar Year : 2024-2025

Explainability of high-dimensional prediction models using neural networks

Non-confidential and publishable report

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Abstract

TO DO

Keywords— Explainable AI, XAI, Anchors, Fairness, Bias, Py4Cast, MeteoFrance, Folktables

Résumé

à FAIRE

Mots clés— IA Explicable, XAI, Anchors, Équité des algorithmes, Biais, Py4Cast, MétéoFrance, Folktables

Acknowledgments

I am deeply grateful to all those who have contributed to the successful completion of this research project during my internship at INRIA Paris and at the Institute of Mathematics of Toulouse (IMT).

.... TO DO

Contents

List of Figures

1 Introduction

The use of machine learning, particularly through deep neural network models, has recently revitalized various fields of mathematical engineering. Notably, the domain of weather forecasting has seen the emergence of new players from the world of machine learning [Lam, 2022], [Kaifeng, 2023], whose predictive model quality approaches that of traditional weather forecasting models. However, models resulting from this work, such as GraphCast, are highly complex and handle very high-dimensional data. As a result, it is currently very difficult to assess the criteria on which they base their predictions, which may limit confidence in their forecasts. These models can be likened to Large Language Models (LLMs), sharing many architectural similarities and exhibiting comparable complexities.

As part of this internship, we will evaluate the relevance of explainable AI methods for high-dimensional AI predictions using MeteoNet data [MeteoNet, 2020] as well as text data in supervised classification tasks. If necessary, we may also adapt these methods to other use cases involving deep neural networks or transformers.

The first stage of the internship will involve familiarizing ourselves with different forecasting models, understanding their underlying mechanisms, and assessing the quality of their predictions. Following an approach similar to [Bommer, 2023], we will then evaluate various explainability methods on data, generalizing the methodology ([Bommer, 2023]). We will develop methods based on concept and anchor creation to assess their stability and determine whether we can uncover learned concepts or mechanisms within the network that help better understand its functioning.

The internship will take place at INRIA Paris in collaboration with the Institute of Mathematics of Toulouse (IMT), under the supervision of Jean-Michel Loubes (INRIA), Benoit Rottembourg (INRIA), and Laurent Risser (ANITI).

1.1 Objectives and division of the report

The primary objective of this research is to conduct a comprehensive analysis of explainable AI methods for complex data, developed at INRIA Paris, and evaluate how to use this different methods among different type of data. Specific objectives include:

- To understand the meteorologic and image data
- To apply Anchors on simpler data, like tabular data
- To understand the difference between Anchors-based, Concept-based explanations
- To develop a way to apply this methods to meteorologic data

This report is structured into the following sections to systematically address the research objectives:

- **Introduction**: Provides background on the challenges of interpretability in high-dimensional models like weather forecasting and introduces the need for explainable AI (XAI) methods to enhance trust and understanding in black-box meteorological models.
- **Literature Review**: Surveys existing XAI techniques (e.g., concept-based explanations, anchors, attention mechanisms) and their applications in climate science and LLMs.
- **Methodology**: Describes the dataset (Titan), models (e.g., deep neural networks, transformers), and XAI techniques tested (e.g., SHAP, LIME, Anchors and alternative approaches).
- **Results**: Presents the findings from the research, including data on the output explanations, efficiency, and scalability of the developed approach.
- **Discussion**: Interprets the results, comparing them with existing forecasting technologies, and discusses the implications of the findings.
- **Conclusion**: Summarizes the key findings, emphasizes the importance of the study, and provides recommendations for future research and practical applications.

2 Literature Review

2.1 XAI and Fairness

To initiate our research on eXplainable Artificial Intelligence (XAI) we chose to get deeper on the Anchors technique (**??**), that is a new technique and under-explored as we found a low number of articles that uses this technique. Reading about Anchors we can notice some aspects that differentiates from SHAP, the state of the art technique in XAI, an important one is the coverage parameter, that shows how much the instance analyzed is generalizable to other instances.

In the domain of bias and bias correction we can see the article (**??**) ...

In the context of this work, we also used a dataset (**??**) to identify unfairness ...

2.2 Weather Forecasting

For the research on weather forecasting we got (**??**) to understand how the predictions are made and how AI can enter in this domain to make faster and more precise predictions. The tool GraphCast for example is presented by (**??**) ...

To understand the data we're using we can understand what generate the AROME images with (**??**) ... an how the AROMA images allied with the UNet convolutional neural networks can be used in practice for example in (**??**).

For the AI model used we focalize on U-NetR++ (**??**) that's the state-of-art on synapse of a neural network.

2.3 LLM and Complex Models

3 Methodology

The first steps of the internship was to get to know the data we would explore. The internship have two main objects, one focused on weather data and the other focused on explainable AI on diverse types of data.

3.1 Fairness Data

In this initial work done with Benoît and Jean-Michel we used the Folktables dataset (**??**) to apply Anchors (**??**) explainable method and try to identify new ways to identify unfairness. The idea to explore Anchors is that this method is under-explored and has an approach different than SHAP, and that can be interesting to detect fairness. Anchors try to find aspects in an individual that can be replicated to others in a local decision, and give the aspects witch anchor that decision when those aspects present.

We took advantage of this behavior to try to find decisions that are based on the sex feature, that means, because the individual was a man or a women, the prediction is always positive or negative. This is really interesting to search for bias in the model prediction.

3.1.1 The Folktables Dataset

For this part of the work we used the Folktables dataset derived from the Census of the United States of America (USA). For manipulating this dataset we used the Python library (**??**) that contains some modules of extraction of the dataset data, focusing on specific target predictions. The target we're using is the Income, so the machine learning model should predict the income of the individual and it will divide True predictions who receives more than 50,000.00 dollars and False who receives less.

3.1.2 Training Data

For our analysis, we utilized data covering the entire United States, as well as from three of the most populous states: California, Texas, and New York. Each subset of data was trained using four widely adopted machine learning algorithms:

- XGBoost (eXtreme Gradient Boosting) – A highly efficient and scalable implementation of gradient boosting, known for its performance in structured data tasks. We leveraged its ability to handle missing values and feature importance estimation.
- Logistic Regression – A classical linear model for binary and multiclass classification. Despite its simplicity, it served as a strong baseline, particularly for interpreting feature coefficients.
- HistGradientBoosting (Skrub's Scikit-learn implementation) – A fast and memory-efficient gradient-boosting variant that bins input features, making it suitable for large datasets while maintaining competitive accuracy.
- Simple Neural Network – A feedforward neural network with a limited number of layers to assess whether deeper architectures could capture nonlinear patterns beyond what tree-based models achieved.

The algorithms were used to classification tasks, to predict the income as higher or lower than 50,000.00 dollars.

In the Table **??** we see the accuracy and fairness metrics, that can be explained as:

- **Accuracy**: The proportion of correct predictions (both true positives and true negatives) among all predictions.
- **Disparate Impact (DI)**: Measures the ratio between the proportion of positive outcomes for the protected group (women) versus the privileged group (men). Values close to 1 indicate fairness, while values below 1 suggest bias against the protected group.

— **Equality of Odds**: Examines whether both groups have equal true positive rates and equal false positive rates. Values closer to 1 indicate better fairness.
— **Sufficiency**: Assesses whether the probability of the true outcome is the same across groups given the predicted outcome. Values closer to 1 indicate better fairness.

Table 1 – Model Performance Comparison Across States (Accuracy and Fairness Metrics)

Model	Training	Testing	Accuracy	Disparate Impact	Equality of Odds	Sufficiency
Logistic Regression	CA	CA	0.56	0.67	0.84	0.95
		USA	0.52	0.66	0.88	0.86
	TX	TX	0.52	0.46	0.65	0.90
		USA	0.51	0.46	0.67	0.95
	NY	NY	0.51	0.66	0.82	0.93
		USA	0.52	0.64	0.86	0.88
XGBoost	CA	CA	0.64	0.72	0.91	0.96
		USA	0.58	0.67	0.92	0.90
	TX	TX	0.60	0.58	0.83	0.93
		USA	0.58	0.58	0.85	0.95
	NY	NY	0.61	0.75	0.92	0.96
		USA	0.57	0.67	0.92	0.90
HistGradientBoosting	CA	CA	0.63	0.71	0.90	0.94
		USA	0.58	0.67	0.92	0.90
	TX	TX	0.61	0.54	0.78	0.96
		USA	0.58	0.56	0.83	0.97
	NY	NY	0.60	0.68	0.89	0.97
		USA	0.58	0.64	0.90	0.91
Neural Network	CA	CA	0.52	0.88	1.03	0.85
		USA	0.46	0.65	0.86	0.86
	TX	TX	0.50	0.61	0.87	0.94
		USA	0.49	0.77	0.96	0.81
	NY	NY	0.51	0.76	0.93	0.92
		USA	0.48	0.66	0.88	0.87

We can see in Table **??** the results comparing the 4 models in the 3 states. In the Figures **??**, **??** and **??** we can see the ROC curves of the models on each sub dataset.

With these plots and metrics we can see the difference of performances between models. In both metrics and ROC curves we can see how XGBoost and HistGradientBoosting outperform the Neural Network, and how the Logistic Regression remains average, but still does not surpass the others.

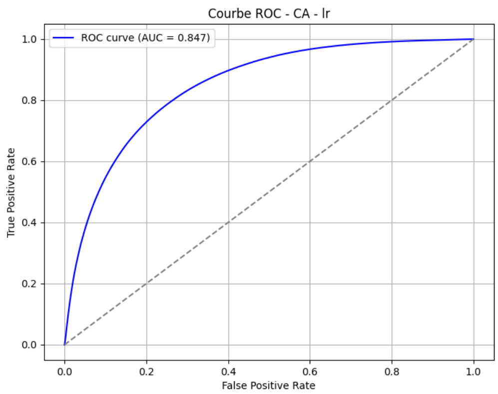
3.1.3 Fairness Metrics

In the Table **??** we see that each ML model was tested for each state and the fairness metrics were calculated for each combination.

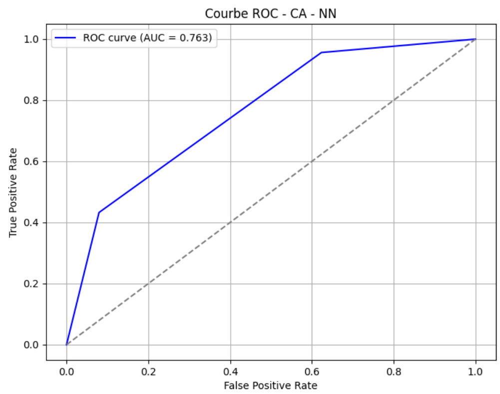
Each model was trained on the train data of the state, as the second column indicates and the metrics were calculated comparing to the test data of the state and the full data of the USA, as indicates the third column.

Note the models with higher accuracy, forth column, as being XGBoost and HistGradient-Boosting. We should now analyse the fairness metrics in the columns five, six and seven.

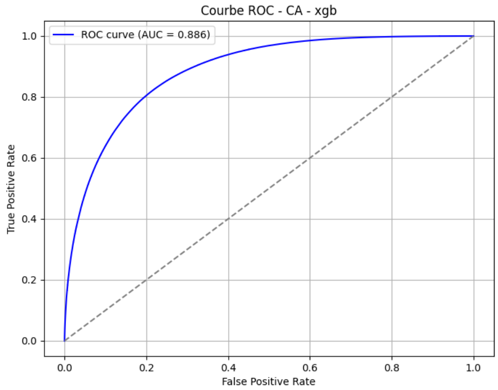
It's important to say that the reference value for each one of these metrics were set by (**??**), which indicates that values above 0.8 or near 1 indicate fairer predictions, while values lower than 0.8 indicate unfairness, in different levels.



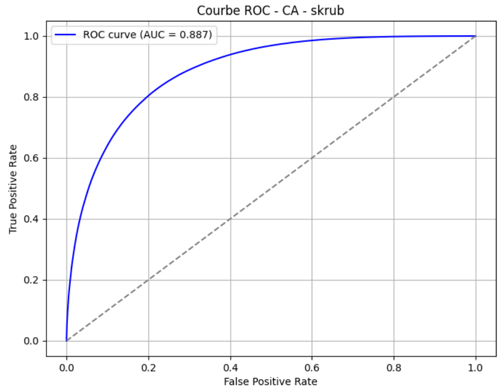
(a) Curve ROC (AUC = 0.847): model = Logistic Regression



(b) Curve ROC (AUC = 0.763): model = Neural Network



(c) Curve ROC (AUC = 0.886): model = XGBoost



(d) Curve ROC (AUC = 0.887): model = HistGradientBoosting

Figure 1 – Comparison of the models trained on the sub dataset of the California state

Note that Equality of Odds and Sufficiency metrics reach higher levels, all of them above 0.8. However, when looking at Disparate Impact (DI), we see a discrepancy from the reference values, them staying in average 2 percentage points lower.

We interpret this low DI as the discrepancy between woman and man that receives more than 50,000.00 dollars, having a disadvantage for woman in this case.

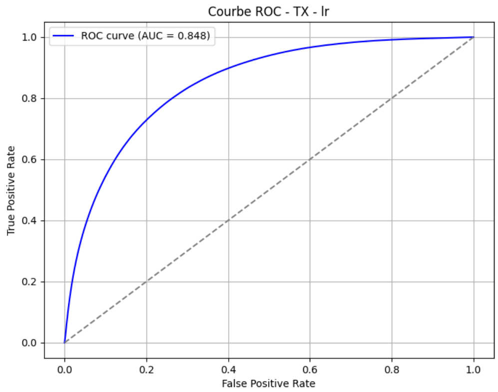
3.1.4 Applying XAI

Having the accuracy of the models and the fairness metrics, we started applying the explainable AI methods on the best ones to try to show the bias with the XAI techniques.

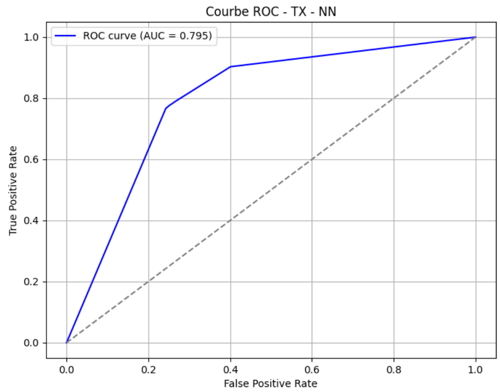
Firstly we generated and exported all the Anchors and SHAP values of the subsets to further analyses. And the following histograms shows the distribution of the XAI methods relative to the 'SEX' variable on the explanations.

The Images **??** and **??** show the distribution of the 'SEX' variables in the Anchors generated for the test data of each state for the models HistGradientBoosting and XGBoost, respectively. Also, we applied filters of precision of the prediction higher than 95%, anchors with less or equal than 3 features (showing compact anchors) and anchors with coverage higher than 10% of the dataset.

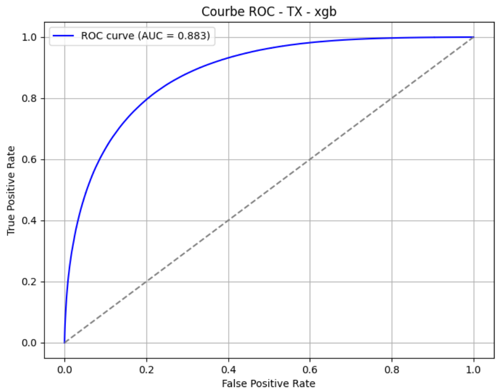
We tried to simulate the same tests on SHAP on the Images **??** and **??**, in the way that we



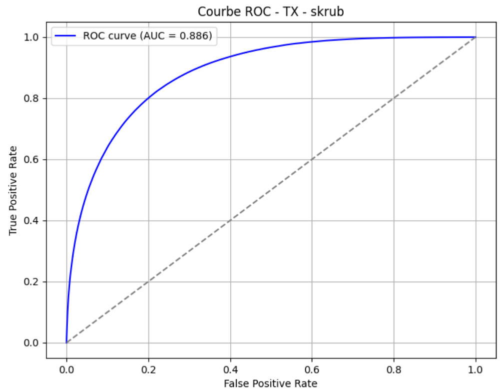
(a) Curve ROC (AUC = 0.848): model = Logistic Regression



(b) Curve ROC (AUC = 0.795): model = Neural Network



(c) Curve ROC (AUC = 0.883): model = XGBoost



(d) Curve ROC (AUC = 0.886): model = HistGradientBoosting

Figure 2 – Comparison of the models trained on the sub dataset of the Texas state

show the distribution of the 'SEX' variables in the positive SHAP values. We applied almost the same filters, apart from the coverage filter because the SHAP values don't have a coverage attribute, and we adapted the filter of number of features to see if the feature 'SEX' was in the first 3 positions of the SHAP values.

Because of what we see in these graphs we can continue to define what we'll call a genred anchor.

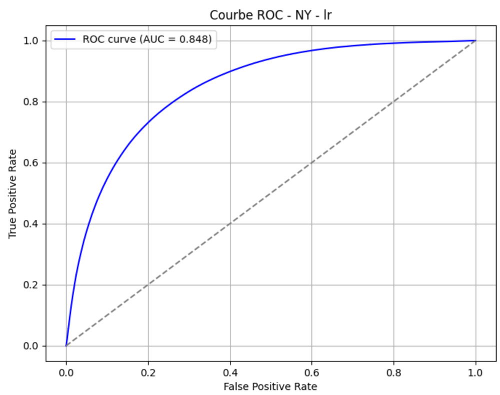
A genred anchor is when the explanation generated contains 'SEX' in the features of the explanation.

It was interesting to see how many Anchors explanations had a genred anchor, that means that the technique identified that feature as decisive to the prediction, meaning that if the value of 'SEX' changes, the prediction changes too. So we decided to investigate it further.

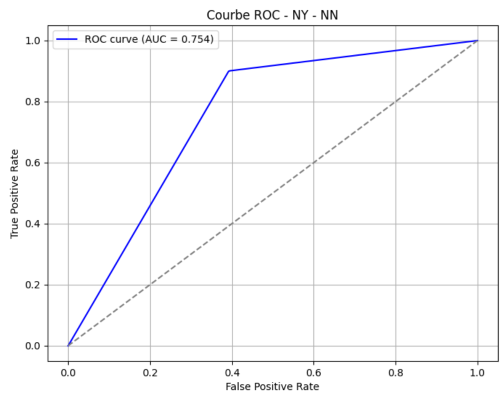
We can notice that the genred anchors are divided manly between between women with a False model prediction and men True prediction. That already show an imbalance in the genred anchors.

3.2 Meteorological Data

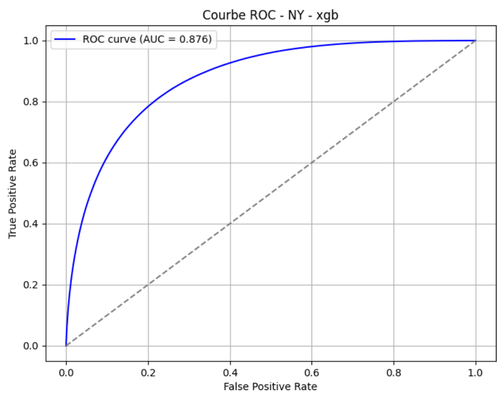
We started by understanding how meteorological data works, and how it is combined to generate a prediction. The first steps were to investigate AROME and ARPÈGE meteorological



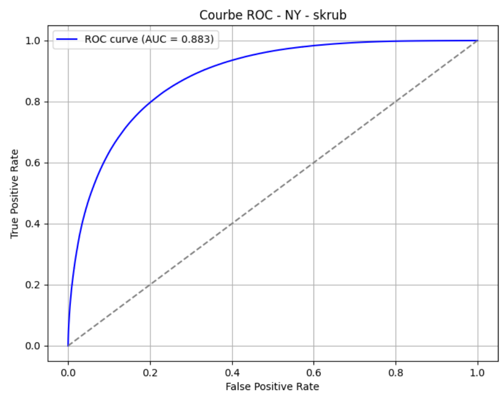
(a) Curve ROC (AUC = 0.848): model = Logistic Regression



(b) Curve ROC (AUC = 0.754): model = Neural Network



(c) Curve ROC (AUC = 0.876): model = XGBoost



(d) Curve ROC (AUC = 0.883): model = HistGradientBoosting

Figure 3 – Comparison of the models trained on the sub dataset of the New York state

data, and we tried to run py4cast for predictions. In second plan as we couldn't run the library, we explored running the UNetRPP with the MFAI library. After, we started applying techniques of eXplainable AI (XAI) in the predictions to get the most important channels or points in the input images that are decisive to the predictions.

3.2.1 The Titan Dataset

Using the Titan (**??**) dataset provided by Méteo France, we could explore the meteorological data and how it is composed. We used for this study the collection of the 2023 year Titan data.

This dataset is organized in folders for each hour, with all of the 37 channels of AROME (**??**) and ARPÈGE (**??**) *.npy* images as described in the Table **??**. In other words, we have a set of these channels for each hour (00h - 23h) of every day of the month and of each month (January of 2023 to December of 2023) of the year.

Each of these channels represent an specific component of meteorological data, and can be resumed in AROME and ARPÈGE channels of temperature, humidity, wind, geopotential in different configurations of pressure level.

The combination of these components can be interpreted and can show that some climatic phenomenon is going to happen. For example it can show that it's going to rain or snow, that it's going to be hot or cold, or that a storm or flooding is happening in the next hour(s).

3.2.2 Training Data

We made some initial analyses in Python notebooks with this datasets, opening the *.npy* images representing the channels and seeing how they are formulated and how we can interpret each channel.

With these data, we used the MFAI (??) Python library, developed by Méteo France, to train a Neural Network (NN) model with the Visual Transformer UNETR++ (??). First we used this NN model to investigate the possible inputs and outputs of a weather prediction. It was helpful to start to understand the complexity of meteorological data and the possibilities to train a model. After this investigation, we could formulate some interesting questions:

— What do we want to predict?
— What should be the input and the output, which channels should be used?
— How we should combine AROME and ARPÈGE data?

After some discussion we defined a direction to follow: to make rain prediction.

That defined, we defined some channels as the priority, the lower atmospheric channels and the ones more directly associated to rain, such as the *aro_r2_2m*, *aro_tp_0m*, *aro_u10_10m* and *aro_v10_10m* channels.

And getting deeper into AROME and ARPÈGE data, we understood the concept of training in the borders. As the AROME data brings the predictions in the fine mesh (high resolution), while ARPÈGE is planetary (low resolution), usually the operational weather forecasting makes the model training with border conditions, that means they use the ARPÈGE is the future time with the AROME in the present to predict the future time. Formalizing the idea we can say that:

Being t the present time, and $t+1$ the future time

— Model training without border conditions :
  If $input = aro_t$, then $output = aro_{t+1} - aro_t$
— Model training with border conditions :
  If $input = [aro_t, arp_t]$, then $output = aro_{t+1} - aro_t$

Training the model with border condition can lead to more precise predictions, as the ARPÈGE brings information from outside of AROME resolution and can predict what's coming in the borders.

3.2.3 Using the py4cast library

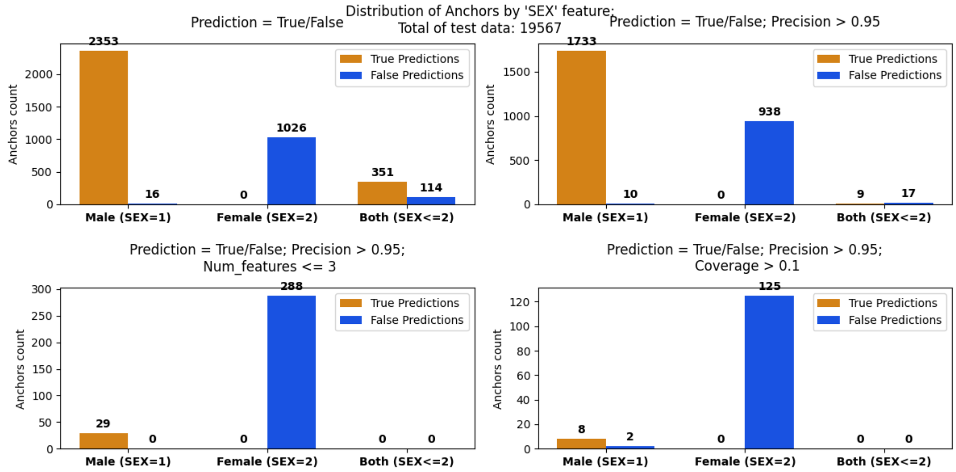
The py4cast (??) library is a framework for weather prediction, that uses AROME and ARPÈGE images as inputs from each one of the channels to generate a prediction in the next 1 hour. The library can be used in many different configurations to make the predictions, using different models, datasets

We worked with Météo France using the library py4cast, developed by them, to train a neural network with the UNetRPP model (??) and the Titan dataset (??) from 2023. This library is very recent and it was really useful for both parts to have an external user to test it. The main objective was to use the library, that already implemented the weather forecast trainings that we needed, but as the documentation didn't consider lots of aspects an external user don't know from the start, we did a lot of debugging to improve the documentation and to turn the library more easily to use by the external user.

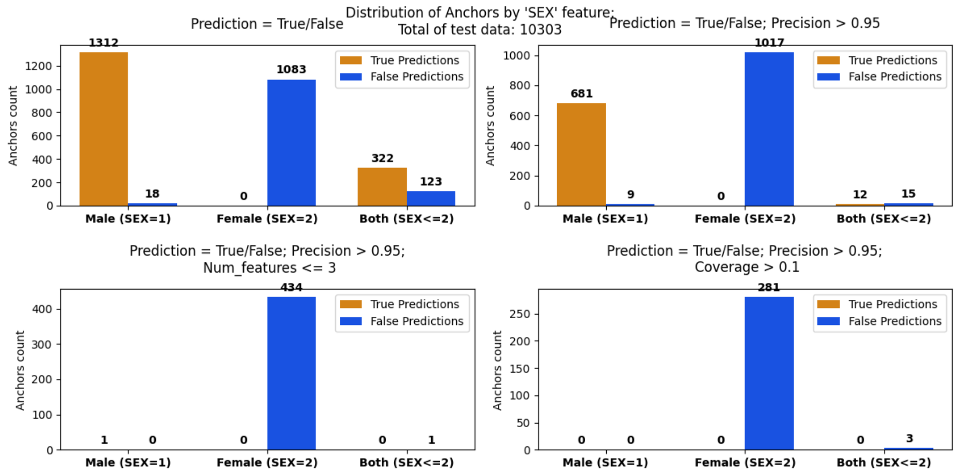
I acted as a type of library tester, reading the documentation and trying to run the UNetRPP trainer, because in practice the workers from Météo France are used to use the library in another environment, that's normally already set up. And after some rounds of debugging, I could run these models and get the images of predictions.

3.2.4 Applying XAI

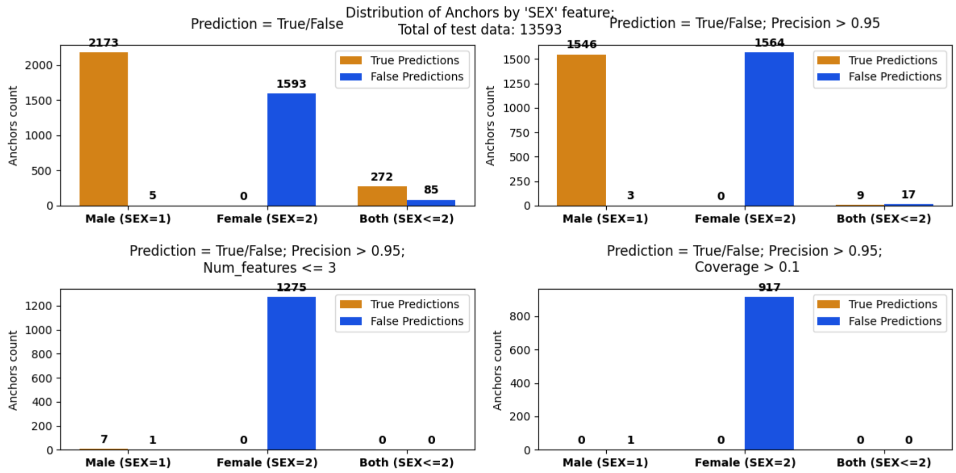
In order to apply XAI we had some problems. XAI techniques like Anchors and SHAP are used for classification models, not regression models like the wether prediction. And these perturbation-based techniques don't take into account many channels of input and specially for meteorologic data could generate images that don't make sense for the context. So we needed to produce a technique that would take this points into account.



(a) State: California

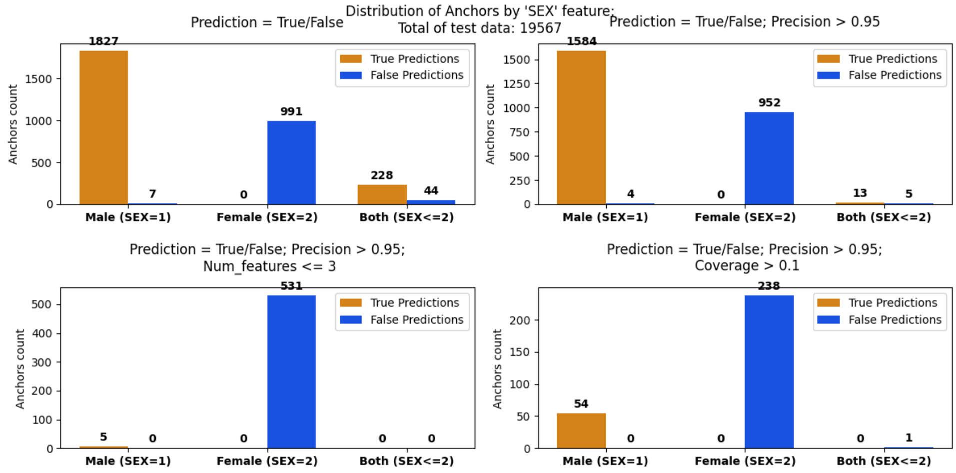


(b) State: New York

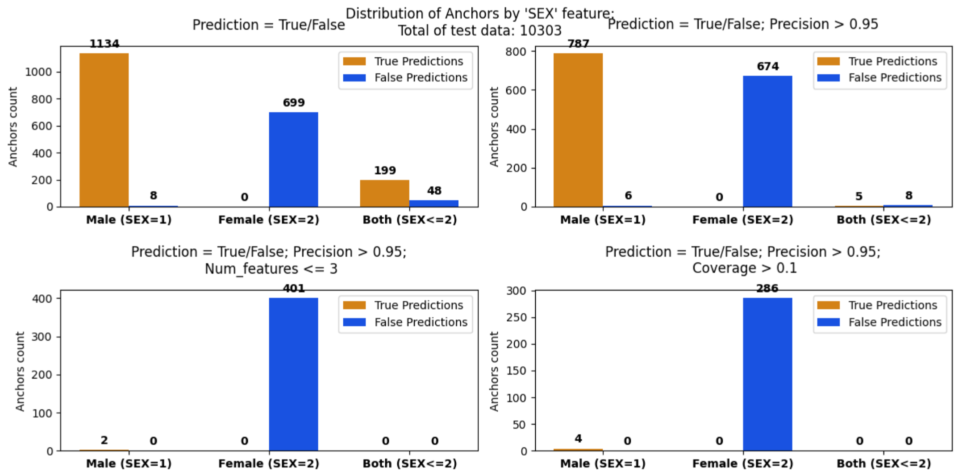


(c) State: Texas

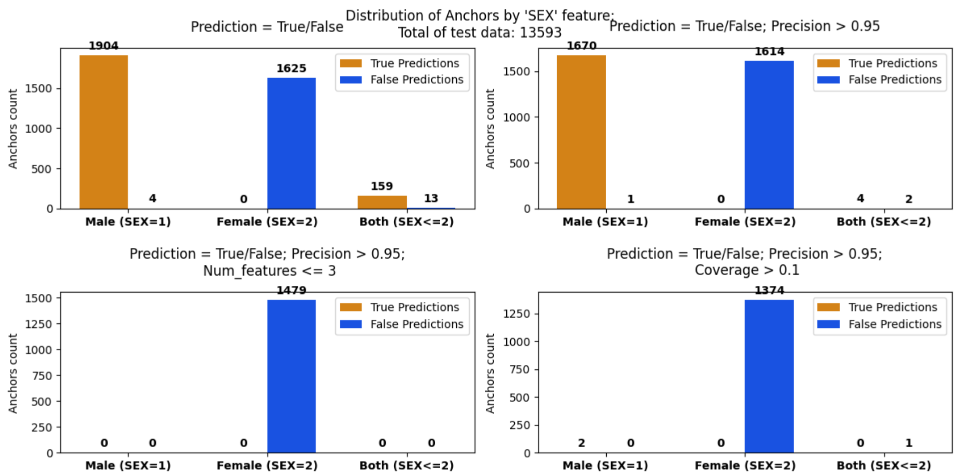
Figure 4 – Comparison of the Anchors sets of the XGBoost model in the 3 states, putting in evidence anchors with the feature 'SEX' in it



(a) State: California

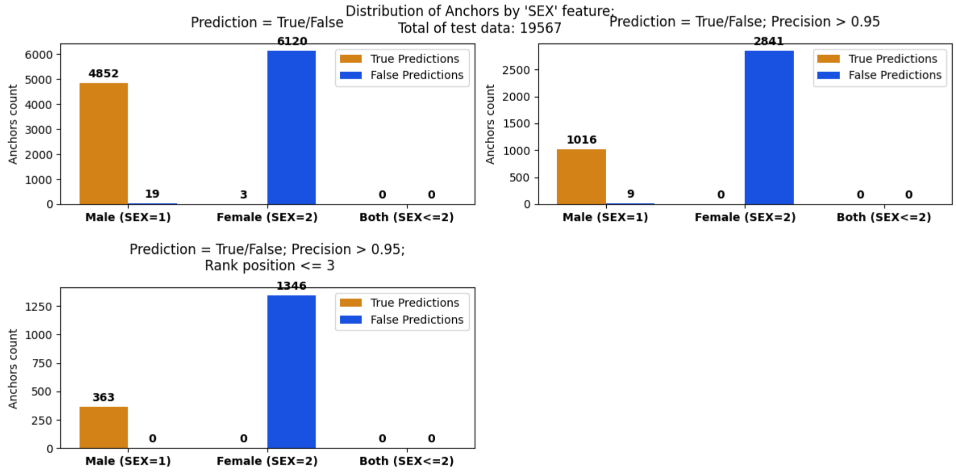


(b) State: New York

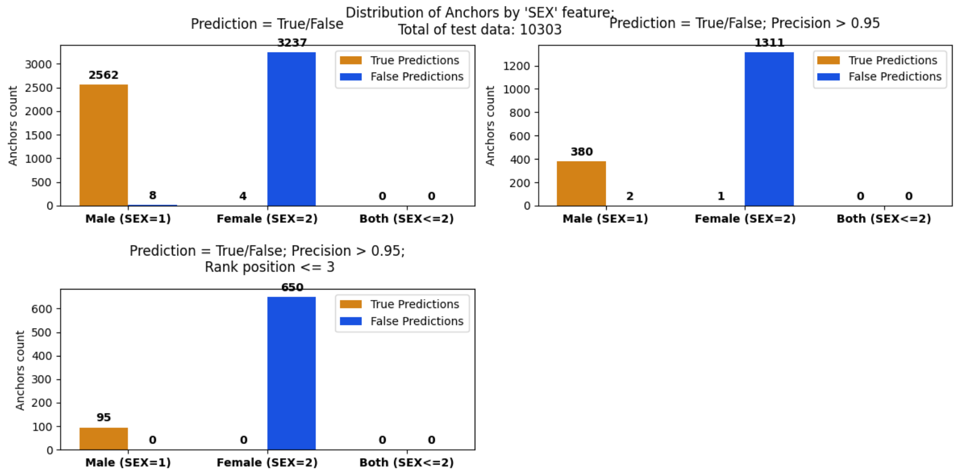


(c) State: Texas

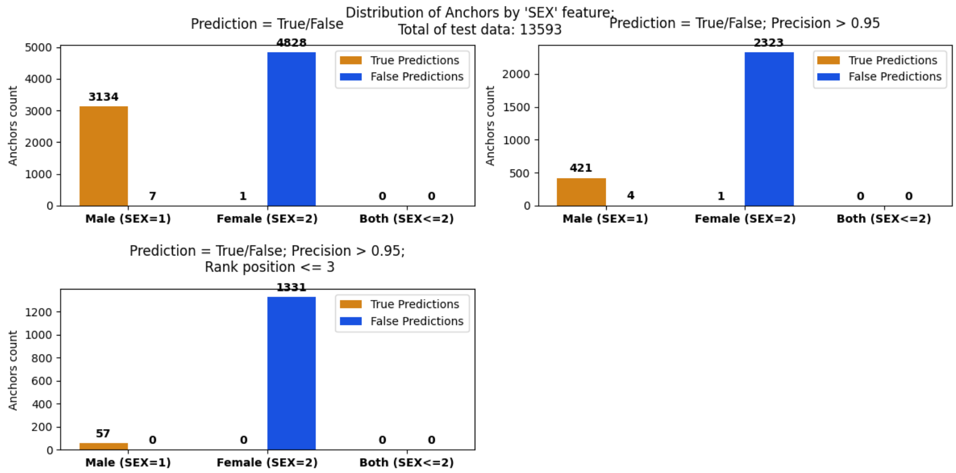
Figure 5 – Comparison of the Anchors sets of the HistGradientBoosting model in the 3 states, putting in evidence anchors with the feature 'SEX' in it



(a) State: California

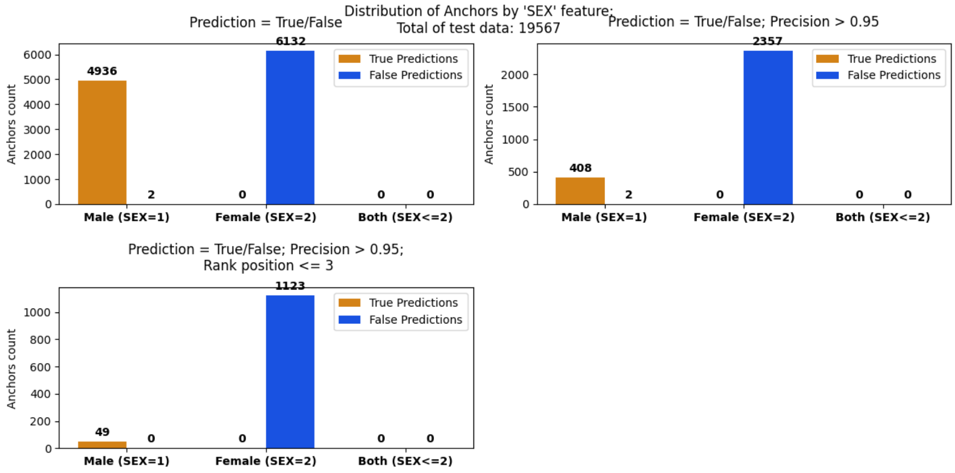


(b) State: New York

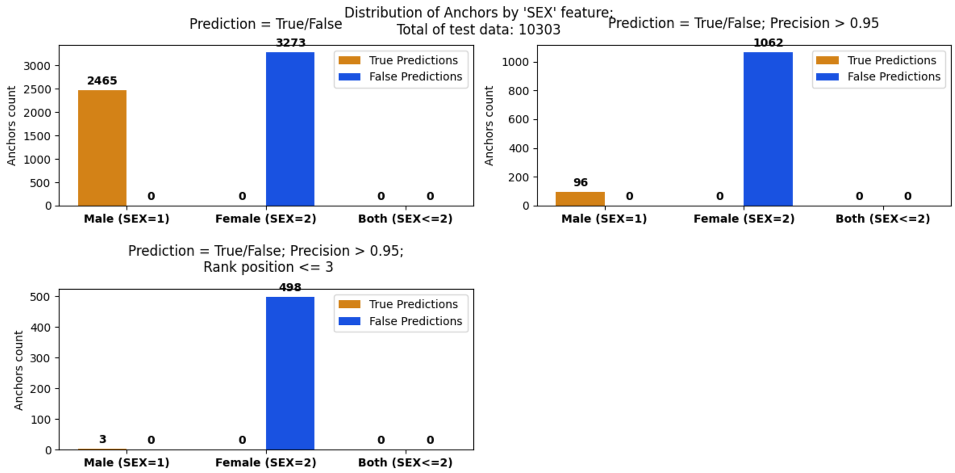


(c) State: Texas

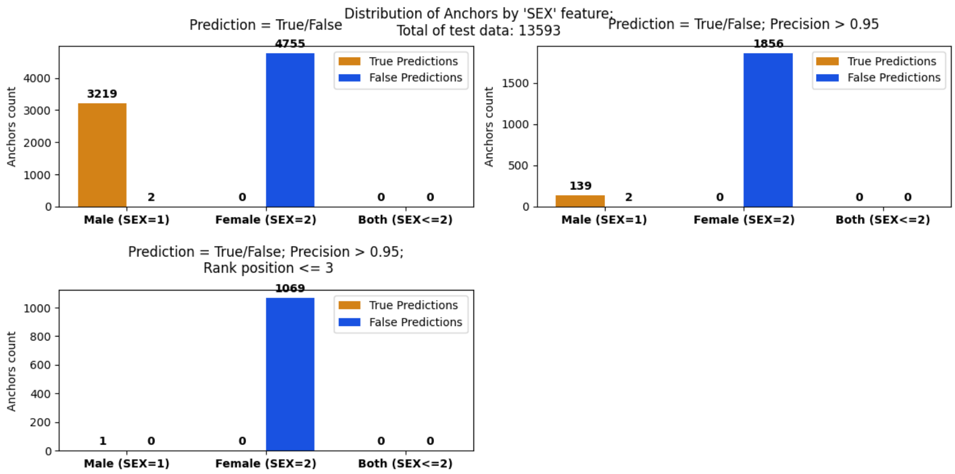
Figure 6 – Comparison of the SHAP values of the XGBoost model in the 3 states, putting in evidence positive explanations with the feature 'SEX' in evidence



(a) State: California



(b) State: New York



(c) State: Texas

Figure 7 – Comparison of the SHAP values of the HistGradientBoosting model in the 3 states, putting in evidence positive explanations with the feature 'SEX' in evidence

Table 2 – Meteorological Data Channels and Their Properties

Channel Name	Description	Altitude/Pressure Level
aro_r2_2m	Arome relative humidity	2 metre
aro_t2m_2m	Arome temperature	2 metre
aro_t_250hpa	Arome temperature	250 hPa
aro_t_500hpa	Arome temperature	500 hPa
aro_t_700hpa	Arome temperature	700 hPa
aro_t_850hpa	Arome temperature	850 hPa
aro_tp_0m	Arome total precipitation	Surface
aro_u10_10m	Arome U wind component	10 metre
aro_u_250hpa	Arome U wind component	250 hPa
aro_u_500hpa	Arome U wind component	500 hPa
aro_u_700hpa	Arome U wind component	700 hPa
aro_u_850hpa	Arome U wind component	850 hPa
aro_v10_10m	Arome V wind component	10 metre
aro_v_250hpa	Arome V wind component	250 hPa
aro_v_500hpa	Arome V wind component	500 hPa
aro_v_700hpa	Arome V wind component	700 hPa
aro_v_850hpa	Arome V wind component	850 hPa
aro_z_250hpa	Arome geopotential	250 hPa
aro_z_500hpa	Arome geopotential	500 hPa
aro_z_700hpa	Arome geopotential	700 hPa
aro_z_850hpa	Arome geopotential	850 hPa
arp_t_250hpa	Arpege temperature	250 hPa
arp_t_500hpa	Arpege temperature	500 hPa
arp_t_700hpa	Arpege temperature	700 hPa
arp_t_850hpa	Arpege temperature	850 hPa
arp_u_250hpa	Arpege U wind component	250 hPa
arp_u_500hpa	Arpege U wind component	500 hPa
arp_u_700hpa	Arpege U wind component	700 hPa
arp_u_850hpa	Arpege U wind component	850 hPa
arp_v_250hpa	Arpege V wind component	250 hPa
arp_v_500hpa	Arpege V wind component	500 hPa
arp_v_700hpa	Arpege V wind component	700 hPa
arp_v_850hpa	Arpege V wind component	850 hPa
arp_z_250hpa	Arpege geopotential	250 hPa
arp_z_500hpa	Arpege geopotential	500 hPa
arp_z_700hpa	Arpege geopotential	700 hPa
arp_z_850hpa	Arpege geopotential	850 hPa

4 Results

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Quisque ullamcorper placerat ipsum. Cras nibh. Morbi vel justo vitae lacus tincidunt ultrices. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. In hac habitasse platea dictumst. Integer tempus convallis augue. Etiam facilisis. Nunc elementum fermentum wisi. Aenean placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

Fusce mauris. Vestibulum luctus nibh at lectus. Sed bibendum, nulla a faucibus semper, leo velit ultricies tellus, ac venenatis arcu wisi vel nisl. Vestibulum diam. Aliquam pellentesque, augue quis sagittis posuere, turpis lacus congue quam, in hendrerit risus eros eget felis. Maecenas eget erat in sapien mattis porttitor. Vestibulum porttitor. Nulla facilisi. Sed a turpis eu lacus commodo facilisis. Morbi fringilla, wisi in dignissim interdum, justo lectus sagittis dui, et vehicula libero dui cursus dui. Mauris tempor ligula sed lacus. Duis cursus enim ut augue. Cras ac magna. Cras nulla. Nulla egestas. Curabitur a leo. Quisque egestas wisi eget nunc. Nam feugiat lacus vel est. Curabitur consectetuer.

5 Discussion

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6 Conclusion

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A Apendix Title

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