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Explainable Artificial Intelligence in Hydrology: Interpreting Black-Box Snowmelt-Driven Streamflow Predictions in an Arid Andean Basin of North-Central Chile

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Abstract: In recent years, a new discipline known as Explainable Artificial Intelligence (XAI) has emerged, which has followed the growing trend experienced by Artificial Intelligence over the last decades. There are, however, important gaps in the adoption of XAI in hydrology research, in terms of application studies in the southern hemisphere, or in studies associated with snowmelt-driven streamflow prediction in arid regions, to mention a few. This paper seeks to contribute to filling these knowledge gaps through the application of XAI techniques in snowmelt-driven streamflow prediction in a basin located in the arid region of north-central Chile in South America. For this, two prediction models were built using the Random Forest algorithm, for one and four months in advance. The models show good prediction performance in the training set for one (RMSE:1.33, R^2: 0.94, MAE:0.55) and four (RMSE: 5.67, R^2:0.94, MAE: 1.51) months in advance. The selected interpretation techniques (importance of the variable, partial dependence plot, accumulated local effects plot, Shapley values and local interpretable model-agnostic explanations) show that hydrometeorological variables in the vicinity of the basin are more important than climate variables and this occurs both for the dataset level and for the months with the lowest streamflow records. The importance of the XAI approach adopted in this study is discussed in terms of its contribution to the understanding of hydrological processes, as well as its role in high-stakes decision-making.

Keywords: Explainable Artificial Intelligence; interpretable machine learning; XAI; iML; hydrology; Chile; streamflow prediction; Elqui River basin

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1. Introduction

Machine Learning (ML) and Deep Learning (DL) algorithms, largely representative of the so-called Artificial Intelligence (AI) [1], are increasingly being used in earth and environmental modeling, including application to the resolution of problems of interest in hydrology and water resources [2–5].

The adoption of AI/ML/DL techniques in the context of water sciences, mostly applied to hydrological prediction and forecasting problems, is part of a growing trend of AI use in Earth System Science, consistent with the so-called Digital Age [6–10].

Although the study and application of AI/ML/DL in the field of hydrology (AI/ML/DL/Hydro) has undergone accelerated growth in the last decade, its adoption continues to be slow compared to other disciplines such as computer science, engineering, mathematics, physics, and astronomy, to name a few [1,11]. According to some authors, this is due to an initial lack of interest in AI and certain techniques associated with information and communication technologies (ICT) that are perceived as if they were a "black box", which has generated a certain degree of skepticism in their actual contribution to the progress of hydrology [12,13]. This initial perception has changed notably as AI/ML/DL has been consolidated as a set of powerful tools to transform large volumes of data—that grow exponentially—into actionable and practical knowledge [9,13]. Indeed, a couple of decades ago, some researchers asked: what does AI contribute to hydrology? [14] Today, as a result of the paradigm shift in science that includes the increasingly predominant role of AI- and ICT-based techniques, the question has been posed in completely opposite terms. That is: what role does hydrological science play in the age of machine learning? [15,16].

Despite the high degree of incorporation of AI/ML/DL into hydrological research and practice, the dilemma regarding the role that these techniques have in the discipline—which, to a large extent, shows a strong predilection for process-based understanding—is not yet resolved. Indeed, some authors state that techniques such as ML are central to the future of hydrological modeling, while others still question whether ML actually has a role in the field [17]. Part of this duality is explained by the central role, as in any scientific discipline, that understanding and explanation have in the progress of hydrological knowledge, "where the ultimate goal is to understand hydrological causality" [18]. However, as the future becomes more uncertain, prediction—precisely one of the most distinctive features of AI/ML/DL—as a scientific value in itself, becomes increasingly important, and is placed, along with understanding, as a key epistemological value for the advancement of the discipline of hydrology [19–21].

It is not strange, then, that recent reviews of the application of AI/ML/DL in hydrology coincide in noting that interpretability, an attribute closely linked to understanding and explanation [22,23], is the most widely criticized aspect regarding the use of AI/ML/DL in the field, since some of these techniques "are particularly difficult to interrogate or justify in physical terms" [2,4,24–27].

The two above-mentioned aspects, predictability and interpretability, the latter of which is considered the basis of scientific understanding, represent a greater challenge due to the so-called prediction/interpretability (also known as performance/transparency, performance/interpretability, accuracy/explainability) trade-off in the AI/ML/DL context. That is, the general idea that indicates the existence of an inverse relationship between the interpretability of black-box models and the degree of precision reached by their predictions, although this relationship is not as simple as has been argued [28–30]. Recent studies on the challenge posed by the prediction/interpretability trade-off [28,29,31] and its explicit incorporation into hydrological modeling show that this is a hot topic and therefore transcendental in the discussion on the role that AI/ML/DL has in current hydrology and will continue to have in an increasingly digitized world [32–34].

In this regard, some authors state that integrating theoretical or disciplinary knowledge aspects with data-driven techniques, an approach known as theory-driven or hydrologically informed machine learning, it is the only "way that we can take full advantage of machine-aided knowledge discovery and advance our understanding of physical processes" [35]. Contrary to that statement, a new and emergent discipline recently adopted in the field of hydrology, known as Explainable Artificial Intelligence (XAI) or Interpretable Machine Learning (iML) [36–38], can provide Machine Learning with more tools to address the prediction/interpretability trade-off in AI-based hydrological research and, in that way, contribute to the progress of hydrological understanding.

However, the adoption of XAI/iML as a complementary discipline to the exponential growth that AI/ML/DL is experiencing in the hydrological field shows important challenges to date. One challenge relates to the heterogeneous distribution, on a global scale, of AI/ML/DL in hydrological research. Figure 1, for example, shows that although AI/ML/DL/Hydro has grown exponentially in recent decades (Figure 1a), countries of the southern hemisphere, apart from Australia, still contribute a very low or even no contribution to the development of the discipline (Figure 1a).

The situation is more unfavorable in the case of XAI/iML in hydrological research (XAI/iML/Hydro), where there are a small number of published articles compared to AI/ML/DL/Hydro in the same period (Figure 1b) and where only a few countries have contributed to XAI/iML research in the field (Figure 1c); none of them, apart from Australia, belong to the southern hemisphere.

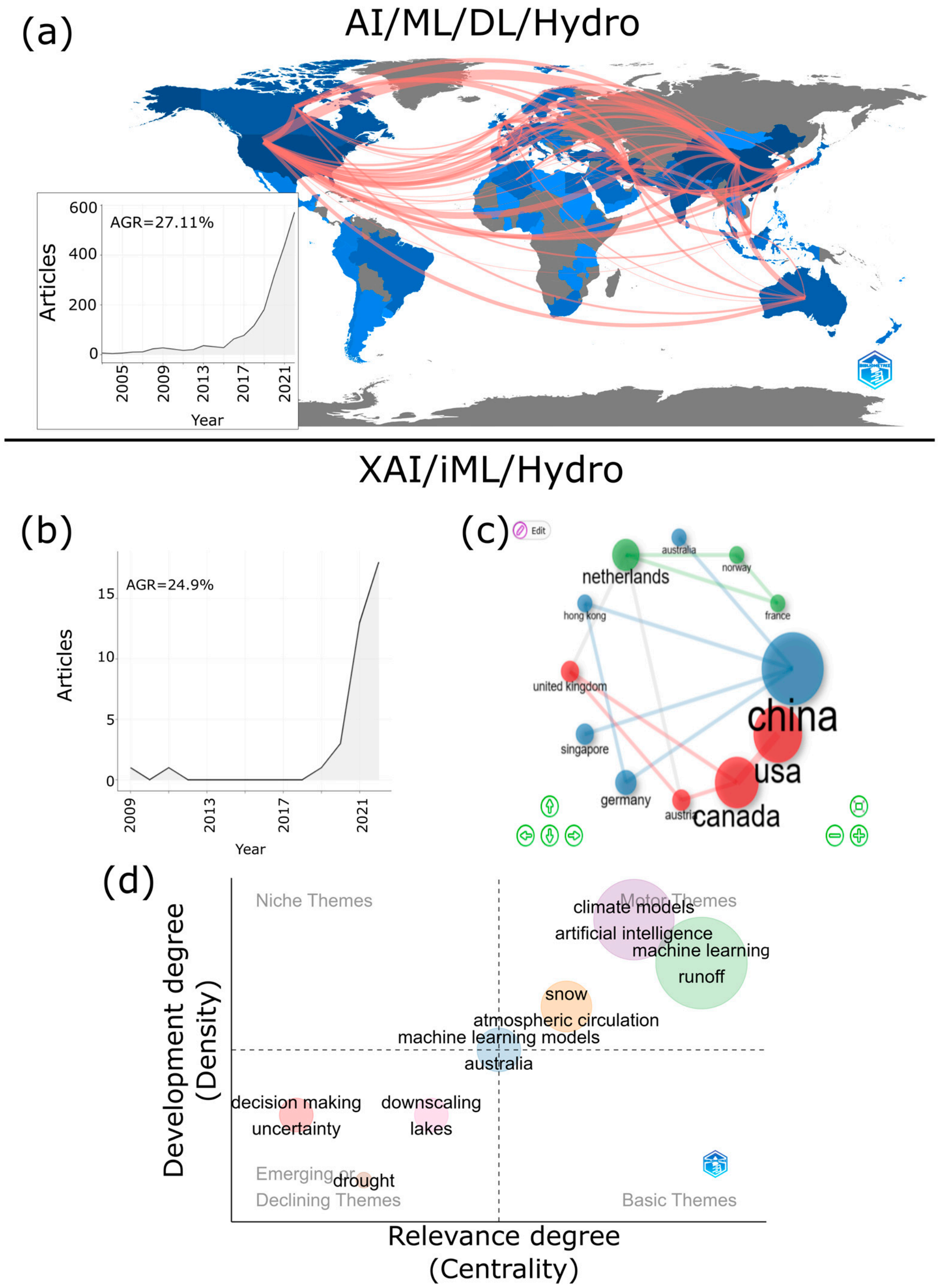

Figure 1. Descriptive statistical plots of AI/ML/DL and XAI/iML hydrological research during 2003–2022. (**a**) Collaboration World Map and Average Growth Rate (AGR) plot for AI/ML/DL; (**b**) Average Growth Rate (AGR) plot for XAI/iML; (**c**) Collaboration Network for XAI/iML; (**d**) Thematic map of XAI/iML. Al plots were generated with the R package bibliometrix [39] using the procedure explained in Appendix A.

Another important challenge of XAI/iML/Hydro is the need to expand research topics to fill knowledge gaps that have not been sufficiently addressed. Thus, for example, Figure 1d shows that the motor themes of XAI/iML/Hydro (first quadrant, top right), that is, themes that are well-developed and crucial for structuring a research subject [40], are currently related to topics such as climate and runoff models (terms such as river, soil moisture, water management, hydrological modeling, streamflow, and flood are subsumed under these two labels). In turn, topics such as water quality, drought or lakes are considered emerging issues (third quadrant, bottom left), implying that they are minimally developed and marginal. The graph allows us to verify that research areas such as seasonal streamflow prediction or snowmelt-driven streamflow prediction in arid regions have not yet been addressed within XAI/iML/Hydro, despite the progress that AI/ML/DL/Hydro has experienced in those research areas. This suggests that there is still room to contribute to filling these gaps with new research in the above-mentioned themes.

Based on the above considerations, this study aims to contribute to the progress of XAI/iML/Hydro with regard to snowmelt-driven streamflow prediction in a basin placed in the southern edge of the Chilean Atacama Desert in South America, an area highly prone to water scarcity and water stress [41], where the need to improve water availability prediction is an urgent and permanent requirement for water resource management. Specifically, this study deals with the application of XAI/iML techniques to the interpretation of snowmelt-driven streamflow prediction in an Andean basin of semi-arid north-central Chile. The study is justified as the selected basin has been affected by a megadrought that has extended over the last decade [42] and its position in the arid zone of the country makes streamflow prediction difficult and prone to large numbers of errors using conventional statistical methods [43]. In this context, an aspect not explored to date is the incorporation of hydrometeorological predictors outside the basin boundaries (e.g., precipitation and streamflow records from stations placed in the basin). Thus, the present study hypothesizes that the inclusion of variables from the vicinity of the basin may have not only predictive but also interpretative importance regarding the outputs of the prediction model. The use of XAI/iML, together with a black-box ML method, allows us to address the prediction/interpretability trade-off mentioned previously with the aim of increasing the prediction accuracy without sacrificing its interpretability.

Finally, the main findings of this study are complemented with a general discussion of the role that XAI/iML could have in hydrological research and practice, in which the authors argue the two main reasons that greater adoption of XAI/iML is necessary in hydrological research. These reasons are (a) its contribution to the progress of hydrological understanding and (b) the role of accountability in the adoption of AI/ML/DL-based hydrological solutions in a context of growing public and political scrutiny and regulatory control.

2. Materials and Methods

2.1. A Case of XAI/iML Application to Prediction of Snowmelt-Driven Streamflows in a Basin of the Semi-Arid Region of North-Central Chile

As an example of XAI/iML application in the hydrological prediction context, the prediction of monthly snowmelt-driven streamflow in the Elqui River basin (ERB), located in the semi-arid region of north-central Chile, was selected as a case study. The prediction was performed using regression models constructed with Random Forest [44], an ML algorithm categorized as a black box [45,46]. The models were built to predict monthly streamflow at two lead times: one and four months in advance with respect to the prediction month (August), consistent with the official procedure adopted for monthly streamflow estimation in the study basin by the General Water Directorate of Chile (GWD). It is recognized that in the past such forecasts had high error levels in the study area [43]. An explanation for this low level of performance could be associated with the use of conventional statistical models with a high degree of transparency but very low predictive performance. Thus, the case study adequately represents the prediction/interpretability trade-off problem discussed in this paper. Improving predictive performance without sacrificing interpretability is key in the search for new reliable forecasting tools, which could also be subject to intense public and political scrutiny due to the effects of forecasting on water management in the basin [47], especially in a context in which the ERB is affected by harsh megadrought conditions that have dragged on for more than a decade [42].

2.2. Study Area

The Elqui River basin is one of the main exorheic basins that make up the Coquimbo Region, north-central Chile. It is located in the Elqui Province, (29°35′ and 30°20′ S, 71°18′ and 69°55′ W), covering an area of 9826 km^2.

The ERB is composed primarily of 4 neighboring sub-basins (Lower Elqui River, Middle Elqui River, Claro River, and Turbio River), with the Río Elqui en Algarrobal (Q_IV_RElquiMedio_Alg) stream gauge station being the monitoring point at which the official prediction of monthly streamflows for the September–March period, coinciding with the snowmelt season, is performed. Figure 2 shows the location of the basin and neighboring basins, as well as the locations of the stream and rain gauge stations, snow courses, and points of interest considered in this study.

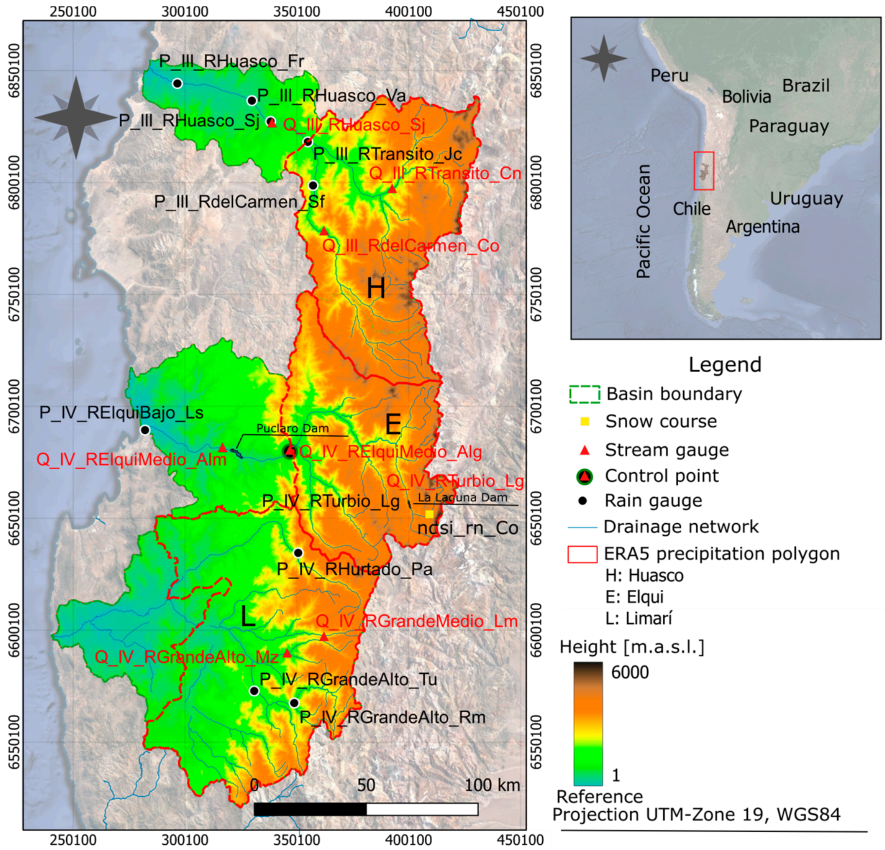

Figure 2. Location map of the Elqui River basin, neighboring basins, and points of interest. Only the names of stations and points of interest in the vicinity of ERB have been placed on the map and labeled.

From a hydrological perspective, precipitation in the ERB presents marked seasonal and interannual variability, with greater precipitation during the wet seasons of autumn and winter (MJJA) and scant precipitation during the rest of the year. The ERB drainage network presents a water regime marked by snow and rainfall in the mountains. The Elqui River, the main stream of the basin, receives contributions from the Turbio and Claro rivers, both from the easternmost region of the basin, in the Andes Mountains.

Regarding the estimated mean monthly streamflow of the Elqui River, at the height of the Río Elqui en Algarrobal station (Q_IV_RElquiMedio_Alg, 760 m.a.s.l.) (see Figure 2), which is the monitoring point used for prediction, the maximum value is presented during the months of December and January, with around 20 m^3/s on average, while the rest of the year the values fall to 10 m^3/s on average [48]. Figure 3 shows the boxplot of monthly streamflow at Río Elqui en Algarrobal stream gauge station, used as the monitoring point for streamflow prediction.

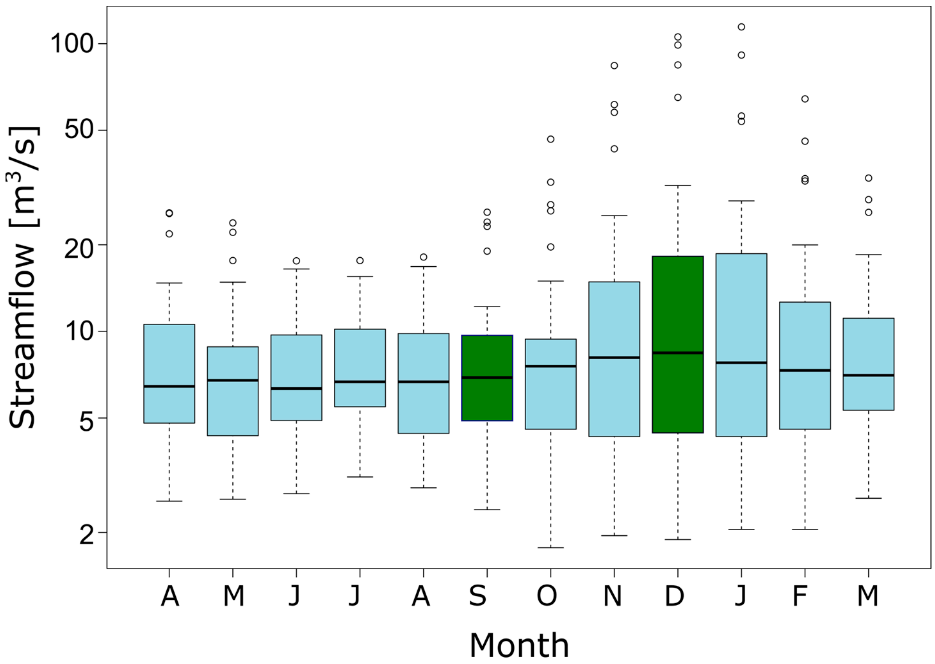

Figure 3. Boxplot of monthly streamflow at Río Elqui en Algarrobal stream gauge station. Boxplots of the months used for prediction are highlighted in green. Vertical axis is plotted in log scale.

2.3. Data Sources and Analysis Tools

Table 1 shows the data sources used. Details regarding the collection and treatment of each of the variables have been described in a previous work [48]. In summary, the main treatment was applied only to streamflow and precipitation variables, not to the variables obtained from gridded sources or those generated with ERA5 (see Table 1). Thus, the treatment included, for the streamflow and precipitation variables, the collection of daily data, analysis of missing and outlier data, elimination of data with a high percentage of missing data, the filling in of missing values using the R package missRanger R [49] and the aggregation of monthly values.

Table 1. Description of main data sources.

Type of Data Source	Data Category	Index or Variable	Symbol in Database	Main Source
Oceanic–Atmospheric	El Niño	El Niño 3.4 SSTA Niño 1.2 SSTA	SST_34 SST_12	HadISST, KNMI Climate Explorer and Met Office Hadley Center NOAA/NCEP/CPC
	Antarctic Oscillation	Antarctic Oscillation index Southern Annular Mode SLP	SAM_Z700 SAM_SLP	Natural Environment Research Council (NERC)
	Geopotential height	Subtropical 500 hPa GH Amundsen Bellingshausen 500 hPa GH	Z500_sub Z500_mid	NCEP/NCAR Reanalysis V1 NCEP/NCAR Reanalysis V1
	Pacific Decadal Oscillation	PDO Index	PDO	Joint Institute for the Study of the Atmosphere and Ocean (JISAO)
	Niño Modoki	El Niño Modoki Index	EMI	Japan Agency for Marine-Earth Science and Technology (JAMSTEC)

Table 1. *Cont.*

Type of Data Source	Data Category	Index or Variable	Symbol in Database	Main Source
	Southern Oscillation	Southern Oscillation Index	SOI	NOAA/NCEP/CPC
	Maden Julian Oscillation	Maden Julian Oscillation	MJ for each phase [1,. . .10]	KNMI Climate Explorer and NOAA/NCEP/CPC
	Subtropical Southwest Pacific SST	Subtropical Southwest Pacific SST index	SST_SSP	NCEP/NCAR Reanalysis V1
	Streamflow	Stream gauge monthly streamflow	Q_x_Ry_z: where x: region y: name of river z: name of place	General Water Directorate of Chile
	Precipitation	Precipitation record	P_x_Ry_z: where x: region y: name of main river z: acronym of rain gauge name	General Water Directorate of Chile
	Grid-based precipitation	ERA5 monthly precipitation	P_ERA5_i: where i: name of polygon location	ERA 5 Reanalysis
	Snow cover	Normalized Difference Snow Index (NDSI)	ndsi	Climate Engine

The prediction (regression) models were built in the RStudio integrated development environment based on R language v4.0.5 [50]. The packages used included caret v6.0-42 [51] for model construction, Boruta v8.0.0 [52] for attribute selection, DALEX v2.4.2 and DALEXtra v2.2.1 [53,54] for model interpretation, and tidyverse v1.3.1 [55] for general database management.

2.4. Procedure

The general procedure is described in Figure 4. All the records described in Table 1 were aggregated to a monthly scale to produce a reliable record period of 41 years (1980–2020). The 2020 record was left out of this database in order to use it as an instance of local model interpretation, such that the final database for regression model construction had a total of 40 instances and 680 attributes (predictors), all numerical. The initial set of predictors was reduced sequentially through (a) elimination of streamflow and precipitation attributes outside the ERB vicinity (outside of the Huasco, Elqui, and Limarí basins), (b) elimination of minimum variance attributes (using the "nearZeroVar" function of the "caret" package with freqCut = 30/10 and uniqueCut = 25), and (c) elimination of attributes with high correlation (using the "findCorrelation" function of the "caret" package with cutoff = 0.8), and (d) standardization (mean = 0, SD = 1). The response variable (streamflow) was used in its original form, and no transformation (c.a. log-transformation) was adopted prior to the assessment of prediction performance and the interpretation analysis [56].

The study objective was defined as the comparison of two prediction models: for one and four months of lead time with respect to the prediction month, consistent with the official methodology currently used by the GWD. From the reduced database, an attribute set was selected for each prediction model with the Boruta algorithm (with default arguments), recognized for its high performance in such tasks [57–59].

Finally, the selected attributes in each model were combined to create a single attribute pool to use in the construction of the two regression models. The models were constructed in Random Forest, using R's ranger v0.13.1 implementation [60]. For the validation, the repeated k-fold cross-validation (args: number = 5, repeats = 10) was used instead of the traditional hold-out partition because it "can provide a more stable estimate of prediction accuracy, as compared with simple k-fold CV," which is highly advantageous for ML applications with small samples where it is not desired to affect the model validity estimation performance [53,56,58,61,62].

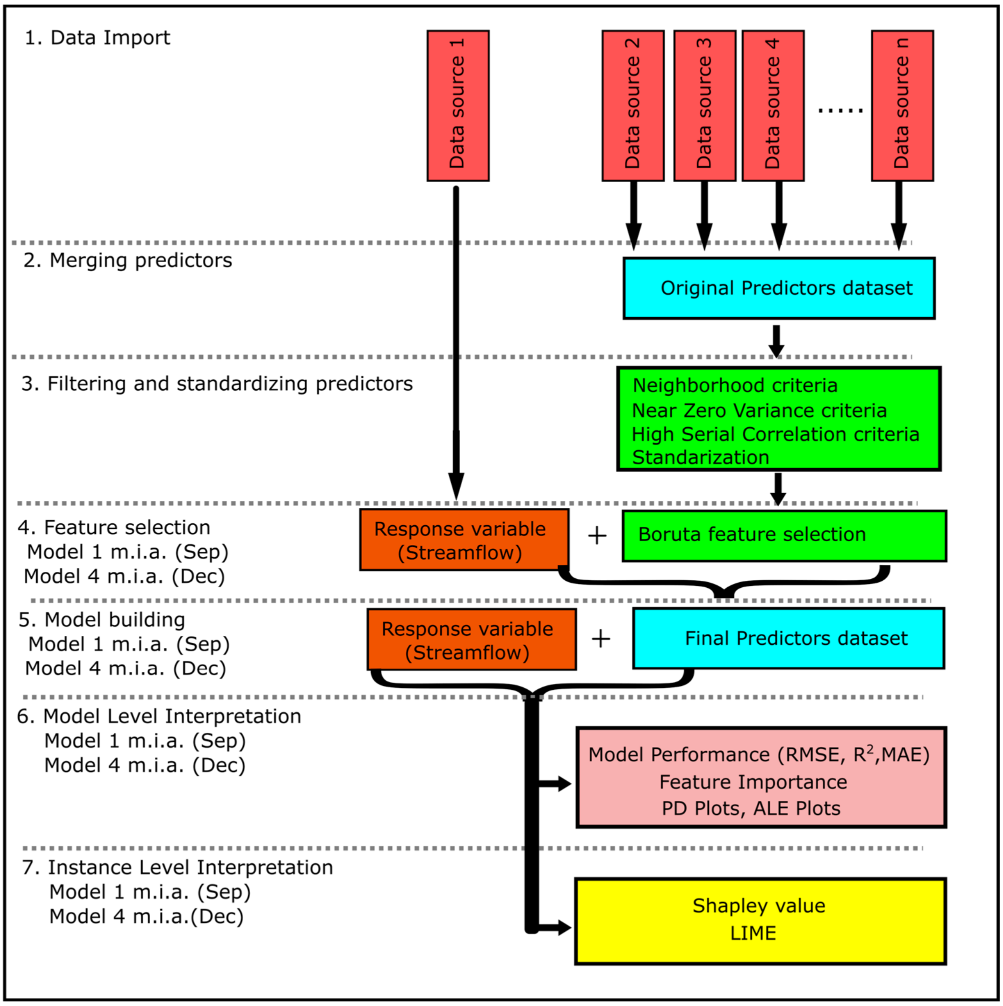

Figure 4. Data pipeline for snowmelt-driven streamflow prediction in the study basin.

For assessment of the prediction performance, the RMSE, R^2, and MAE metrics were used. For the interpretation of results at model (dataset) level, the variable importance (VI) [53,56], partial dependence plot (PDP) and accumulated local effects plot (ALE) techniques were used, while for local (instance)-level interpretation for the year of the series with the lowest streamflow (2020), the Shapley value (SHAPv) and local interpretable model-agnostic explanation (LIME) techniques were used [53,56]. Variable importance resides in the idea that if a variable is important it can be expected that, after permuting the values of the variable, the model's performance will worsen. The amount of change in the performance is a measure of the importance of the variable [56]. Partial dependence plot shows how the expected value of model prediction behaves as a function of a selected explanatory variable [56,63]. Accumulated local effects plot, an unbiased alternative to PDP, describes how features influence the prediction of an ML model, on average [64].

The Shapley value calculates the contribution of each attribute to the predicted value. Put another way, "The value of feature j contributes ϕj to the prediction of this particular instance, compared to the average prediction for the data set."[64]. Finally, the idea behind LIME is to locally approximate a black-box model using a simpler transparent model which is easy to interpret. In the implementation adopted in this study, the surrogate local model corresponds to a weighted LASSO lineal regression model [56].

3. Results

3.1. Model (Dataset)-Level Interpretation

The AI/ML/DL model interpretation process begins at model performance level, "as interpretation can only be as good as its underlying model" [62]. Accordingly, Table 2 presents the performance metrics of the streamflow prediction models for 1 month in advance (m.i.a.) (September: Sep) and 4 m.i.a. (December: Dec), respectively.

Table 2. XAI/iML techniques potentially applicable to the field of hydrology.

Model	RMSE		R^2		MAE	
	Train	Cross-V	Train	Cross-V	Train	Cross-V
1 m.i.a. (Sep)	1.3313	2.5905	0.9421	0.8530	0.5517	1.8426
4 m.i.a. (Dec)	5.6747	12.1906	0.9495	0.7282	1.5152	8.3943

The results show high performance (i.e., R^2 = 0.94) for the sample used for training, and lower performance (i.e., R^2 = 0.85) for the validation sample (obtained by CV) in the different metrics for the 1-month-in-advance model (Sep). The 4-months-in-advance model (Dec) presents high performance (i.e., R^2 = 0.95) for the training sample and lower performance (i.e., R^2 = 0.73) for the validation sample (obtained by CV). The results are consistent with other streamflow prediction studies in the same basin, although they have different methodologies in terms of predictive performance. Likewise, they are consistent with the fact that predictive performance in the ERB tends to decrease as the prediction lead time increases [65]. In addition, the results are positive compared to those obtained historically on an official basis by the General Water Directorate of Chile in this basin, as studies indicate that no forecast performed in northern Chile has entered the "good forecast" category [43]. These results suggest the possibility of comparing, in the future, a set of ML/DL models with different levels of complexity, taking account for the fact that, within the XAI/iML framework, models with approximately equally predictive performance could give rise to different interpretations.

Regarding the most important variables for prediction, Figure 5 shows the mean importance of the variables by prediction model.

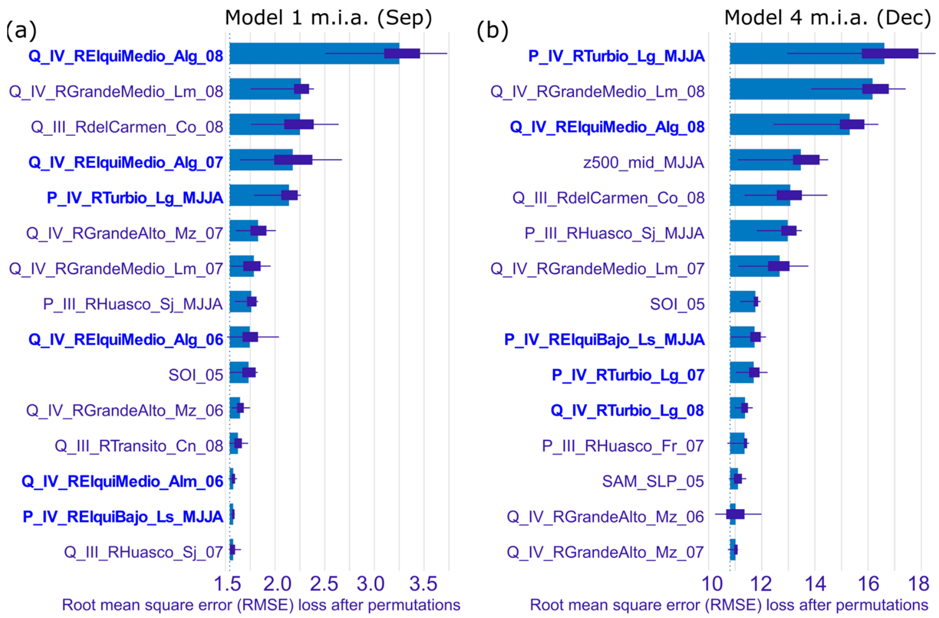

Figure 5. Permutation-based variable importance by prediction model: (**a**) Model for 1 month in advance (m.i.a.) (Sep) and (**b**) Model for 4 months in advance (m.i.a.) (Dec). Names of stations located inside ERB are shown in bold.

As seen in the graph, the order of variable importance is not the same in the two models. In the case of 1 month ahead (Sep), the four most important variables are: streamflow at the Río Elqui en Algarrobal station (Q_IV_RElquiMedio_Alg_08), streamflow at the Río Los Molles en Ojos de Agua station (Q_IV_RGrandeMedio_Lm_08) in August, streamflow at the Río Carmen en el Corral station (Q_III_RdelCarmen_Co_08) in August, and streamflow at the Río Elqui en Algarrobal station (Q_IV_RElquiMedio_Alg_08) in July. In the case of 4 months ahead (Dec), the four most important variables are cumulative precipitation in the rainy season (MJJA) at the La Laguna Embalse station (P_IV_RTurbio_Lg_MJJA), streamflow at the Río Los Molles en Ojos de Agua station (Q_IV_RGrandeMedio_Lm_08) in August, streamflow at the Río Elqui en Algarrobal station (Q_IV_RElquiMedio_Alg_08) in August, and the 500 hPa geopotential height in the Amundsen–Bellingshausen sector. It is possible to interpret the set of precipitation and streamflow variables in terms of the water status in the ERB vicinity. Climatic variables, which have traditionally been incorporated as predictors of the water regime in a large part of continental Chile [42,66], have less importance, depending on the model. For 1 m.i.a. (Sep), only the Southern Oscillation Index (SOI) for the month of May appears among the 15 most important variables, with very low importance. For 4 m.i.a. (Dec), meanwhile, 500 hPa geopotential height for the rainy season (MJJA) in the Amundsen–Bellingshausen sector appears in fourth place of importance. This finding is consistent with what has been found by other authors who indicate that this variable is associated with the current megadrought conditions affecting a large part of continental Chile [42]. This aspect is important, as December is the month of peak snowmelt in the streamflows in the ERB and, therefore, when the greatest contribution to the cumulative water volume in the basin occurs. In the same model, the SOI for the month of May is less important, which could be explained by the fact that El Niño conditions have lost precipitation prediction ability in central and north-central Chile. Indeed, El Niño has presented less predictive ability in the last decade due to the influence of other ocean climate factors, with the 500 hPa geopotential height in the Amundsen–Bellingshausen sector standing out [42,67].

Figure 6a,b presents the partial dependence plots (PDP), also known as partial dependence profiles, for both models, to show how the expected prediction value behaves as a function of some variable of interest, using the most important variable in each model [56,62,63]. The graphs highlight two important aspects for interpretation: first, it is observed that the individual ceteris paribus (CP) profiles, similar to the individual conditional expectation (ICE) plots, are parallel, which is indicative of an additive model without interaction between predictors, and facilitating extrapolation in the predictor space by making the PDP adequately represent the profile of each instance [56,65,68]. Second, the graphs show that for values between −1 and 1 SD from the predictor mean, the estimated streamflow at Río Elqui en Algarrobal presents a low linear increase, although it is clearly staggered throughout the prediction domain. With predictor values of more than 1 SD from the mean, a faster increase in estimated streamflow at the monitoring station is observed, of up to approximately 2 SD from the mean.

This can be interpreted in terms of thresholds in the predictors that indicate the occurrence of a staggered change in predictor–response relationships, which seems reasonable since hydrological relationships between precipitation and snowmelt-driven streamflows in mountainous areas are generally parameterized in terms of threshold values [68,69]. The foregoing is confirmed by the accumulated local effects (ALE) plots, also called accumulated local profiles, which are shown in Figure 6c,d. The ALE plots in this case have an interpretation similar to that of the PDP, thanks to the lack of interaction between predictors. It is more clearly seen that both models present three predictor–predicted streamflow relationship levels. For 1 m.i.a. (Sep) (Figure 6c), streamflow at the Río Elqui en Algarrobal station (Q_IV_RElquiMedio_Alg_08) in August presents a first level between −1 SD and 0, a second level for values between 0 and 1.3 SD, and a third level for values above 1.3 SD. Meanwhile, for 4 m.i.a. (Dec) (Figure 6d), cumulative precipitation in the rainy season (MJJA) at the La Laguna Embalse station (P_IV_RTurbio_Lg_MJJA) presents a first level between approximately −1 and 0, a second between 0.3 and 1, and a third for values over 1.2 SD.

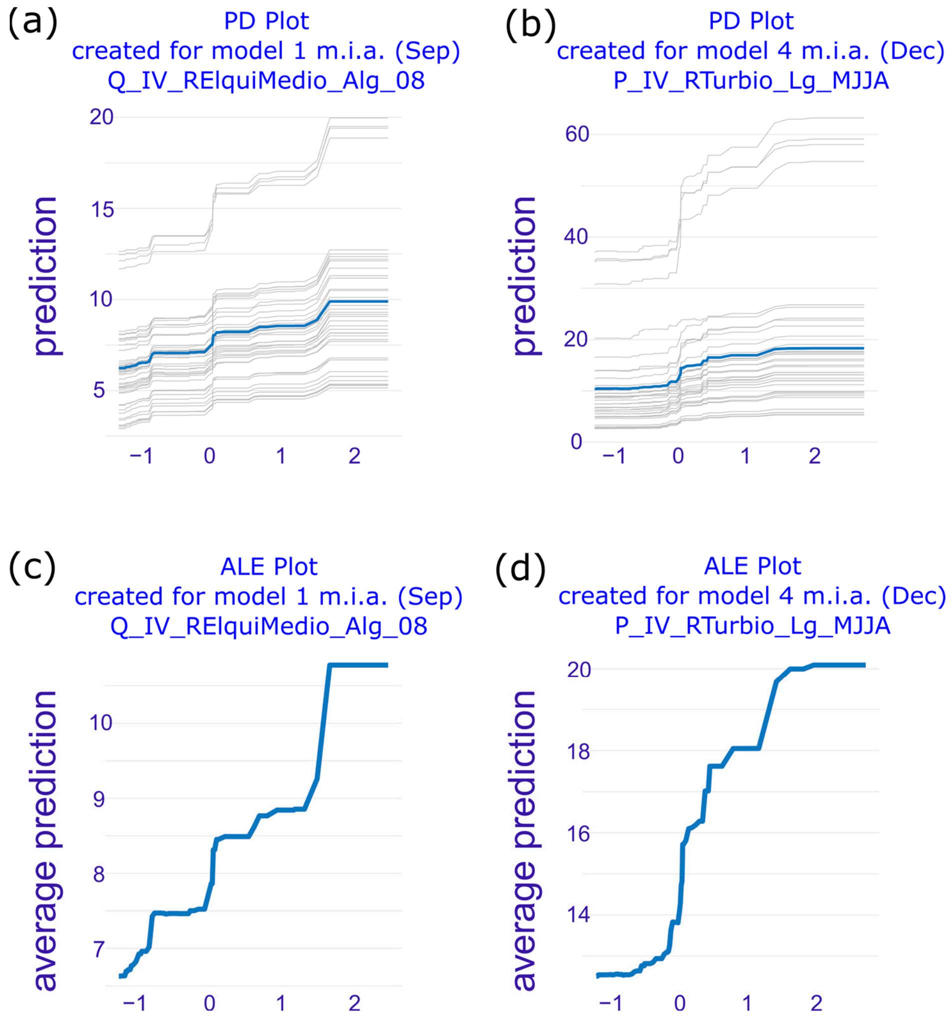

Figure 6. PDP and ALE plots by prediction model: (**a**) PDP—1 m.i.a. (Sep), (**b**) PDP—4 m.i.a. (Dec), (**c**) ALE–1 m.i.a. (Sep) and (**d**) ALE–4 m.i.a. (Dec). m.i.a. = Month(s) in advance.

Thus, ALE plots make it possible to verify that the effect of predictors on forecast streamflow is consistent not only with intuition, but also with what is postulated by the domain knowledge on hydrological relationships in high mountain conditions [68–70].

3.2. Local (Instance)-Level Interpretation

Because the study area has experienced megadrought conditions in the last decade, associated with various factors [42,66,67], it is important to analyze how the selected attributes explain the lower streamflow recorded in the available database. To this end, the September (December) 2020 streamflow was selected as the event to forecast, and the results were interpreted in terms of the Shapley value (SHAPv) and LIME, two of the most-used local techniques for hydrological applications in the XAI/iML context [56,63,64].

Figure 7, below, shows the SHAPv and LIME values for the main variables that explain the September (December) 2020 streamflow. SHAPv assigns each feature an importance value for a particular prediction. As seen in the figure, for September 2020 (Figure 7a) the three most important variables are streamflow at the Río Elqui en Algarrobal station in August (QIV_RElquiMedio_Alg_08), streamflow at the Río Elqui en Algarrobal station in July (QIV_RElquiMedio_Alg_07), and streamflow at the Río Carmen en el Corral (Q_III_RdelCarmen_Co_08) in August. Meanwhile, for December (Figure 7b), the three most important variables are precipitation at the Laguna Embalse station in winter (MJJA) (P_IV_RTurbio_Lg_MJJA), streamflow at the Río Carmen en el Corral station (Q_III_RdelCarmen_Co_08) in August, and streamflow at the Río Elqui en Algarrobal station (QIV_RElquiMedio_Alg_08) in August. Thus, in predictive terms, the water status of the vicinity of the Elqui River basin explains, to a large extent, the minimum streamflow recorded in September (December) 2020. The use of SHAPv, therefore, allows the importance of the selected variables for a particular instance-level prediction to be distinguished from their importance in a dataset-level model.

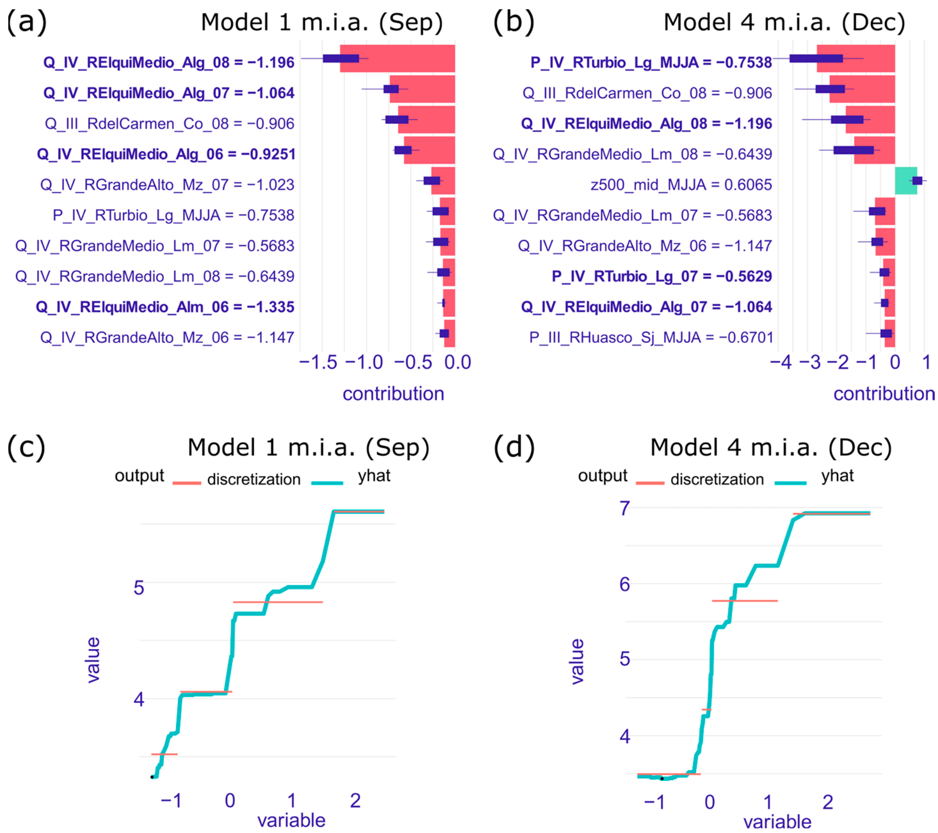

Figure 7. Shapley value and LIME plots based on prediction model: (**a**) SHAPv—September; (**b**) SHAPv—December; (**c**) LIME—September; (**d**) LIME—December. Names of stations located inside ERB are shown in bold.

LIME, meanwhile, is a surrogate model, trained to approximate the predictions of the underlying black-box model to explain individual predictions by learning an interpretable model locally around the prediction [56,64,71]. LIME prediction curves were generated using the main variable in each model obtained by SHAPv. It can clearly be observed that the low estimated streamflow in both months is explained because, in each model, the value of the most important predictor variable was found on the lower predictor–response relationship level.

These findings are important from the perspective of streamflow prediction models for the study area if they are compared, for example, to the official findings of the General Water Directorate of Chile or those of local and research organizations, which base their forecasts on a combination of global climatic variables and exclusively local variables (within ERB boundaries); that is, variables that do not incorporate information from the basin vicinity into the forecasting models [65,72–74]. This can be explained by the role that scientific knowledge and understanding have in hydrological research and practice, in which the variables selected by the analyst are expected to obey some mechanism that is plausible in physical terms; this is typical of the culture some call “data modeling,” the purpose of which is “[t]o extract some information about how nature is associating the response variables to the input variables" [75,76]. By contrast, in a data-driven approach, the variables are selected algorithmically based on the minimization of a loss function. The role of XAI/iML in this context is precisely to generate an explanation, that is, "the process of describing one or more facts, such that it facilitates the understanding of aspects related to said facts" [77].

4. Discussion

Even though recent studies have shown the utility of XAI/iML in hydrological research, such as in the interpretation of black-box prediction models in tropical areas of Brazil in the southern hemisphere [78], in the prediction of levels of groundwater in a aquifer in the semi-arid region of the southern United States [79] or in the prediction of groundwater levels in a desert region of China [80], to mention a few, this is the first study, according to the best knowledge of the authors, looking at the application of XAI/iML to snowmelt-driven streamflow prediction in an Andean basin of South America.

The XAI/iML techniques used in this study contributed to the interpretation of the black-box model outputs in two ways: first, the results allowed us to identify the importance of hydrometeorological variables outside the basin boundaries, which is a novel element of our research, since most of previous research in the study area restricts the set of this type of variables to those located locally within basin boundaries [43,65]. Due to the scarcity of data in most of the South American countries in particular, and in arid and mountain regions, the use of local variables beyond the basin boundaries, as a way of compensating space for time (similar to the idea of "trading space for time" used in regional frequency analysis in hydrology [81]), offers the possibility of improving the performance of predictive models under conditions of data scarcity, which is common in several countries of the southern hemisphere. Second, the results are consistent with hydrological knowledge, regarding threshold values in the relationship between precipitation and streamflow, for example, which reinforces what has been indicated at the beginning of the study, that XAI/iML techniques constitute valid tools for the progress of the discipline in terms of its contribution to hydrological understanding. The above is part of a broader debate regarding the role that XAI/iML and AI/ML/DL have on scientific progress and on high-stakes decision making that may impact society, as described below.

Various authors have addressed the reasons that XAI/iML is considered important and even necessary amid the increasing advancement of AI/ML/DL in today's society. These considerations include the need for transparency, "to trust the model, especially when they are used for high-stakes application" [82]; the need to open black-box models, "not only for acceptability within society, but also for regulatory purposes" [83]; to meet various requirements and address concerns that arise from various domains, including "social, cognitive, philosophical, ethical and legal" concerns [84]; "To facilitate greater human acceptability" of AI-based systems [85]; to address the challenge of greater transparency due to the relationship between transparency and trustworthy AI, the basis for some recent regulations [86]; and "To amend the lack of understanding of AI-based systems, their reasoning processes, and their outputs" [87], to name a few. As stated in a recent study on the matter, "Many further reasons [including legal reasons] of public interest, like fairness or security, as well as business interests like ease of debugging, knowledge retrieval, or appropriate user trust have been identified" [63].

In the hydrology context, unlike the reasons expressed in the general AI/ML/DL community, the main reasons stated by researchers for the incorporation of XAI/iML are related to their contribution to greater understanding of the hydrological process, coinciding with the epistemic value of understanding in the progress of the discipline [18–21]. In the opinion of the authors of this paper, however, the incorporation of XAI/iML into the discipline should involve at least two main reasons based on the factors that have historically shaped the progress of the discipline: technological development and the needs of society [88]. These reasons are: (a) the contribution of XAI/iML to the progress of hydrological understanding in the first place, and (b) accountability in the use of AI/ML/DL techniques in a context increasingly permeated by ethical, political, and regulatory considerations, where AI-based solutions are increasingly more embedded in high-stakes decision-making systems [47,89].

Each of the mentioned reasons is detailed below:

(a) Contribution to the understanding and progress of the discipline: The first reason for which it is considered not only important but also necessary to deepen the adoption of XAI/iML in hydrological research is that this discipline aids in facing the transparency limitations of the black-box techniques that have undergone major expansion in the discipline. This reason is argued by the authors of this paper, contrary to what is stated by those who, regarding the theory-guided approach, indicate that "It is only in this way that we can take full advantage of machine-aided knowledge discovery and advance our understanding of physical processes." [35]. The reasons presented in hydrological applications of XAI/iML to date clearly reinforce this conviction. For example, some of the reasons expressed by researchers for including XAI/iML in their applications of AI/ML/DL are: that interpretable machine learning methods are adopted for better physical understanding [90]; to interpret the optimum modeling and understand how each input variable affects the selected output [80]; to extend the interpretability of machine learning models so the results can be better understood by humans [91]; to show that ML methods can provide accurate predictions for various tasks and that the hydrological processes involved can be interpreted so that results are more understandable to humans [92]; and to overcome black-box model limitations related to practical implications for water resource research [93]. Thus, as stated in other studies, in terms of contribution to the understanding of hydrological processes based on the application of AI/ML/DL, the authors of this paper also "recommend that the hydrological community makes more use of the novel methods of interpretable machine learning" [94].

(b) Accountability in trustworthy AI/ML/DL for high-stakes decision-making systems: The second reason that XAI/iML can contribute significantly to hydrological research and practice, which has been tangentially recognized in the hydrology community, is the importance that ethical and regulatory issues concerning the use of AI/ML/DL overall have taken on [83,85,95–98]. The regulatory aspect has emerged as a natural extension of the ethical debate on AI toward the field of AI governance, the main objective of which is to achieve what has been called Trustworthy AI [99]. Hydrology, a discipline that throughout its history has known how to adapt to the context of technological development and social needs in which it is immersed [88], due to its own evolution, is inextricably linked to human affairs. And while an understanding of the processes and the progress of hydrological knowledge continue to be the main value of the discipline [19–21], the contribution of hydrology to solving the problems of society will require consideration of the ethical issues behind the solutions it provides [18,100]. This idea is reinforced when the discipline itself has explicitly recognized the increasingly substantial role of human–water interactions, and where communication of scientific knowledge and the acquisition of feedback from stakeholders are key factors in the progress of the discipline and its mission to be a "science for solutions" [101]. Various authors have begun to analyze and recognize the ethical and accountability implications brought about by the use of AI/ML/DL in hydrological research (see, for example, a recent discussion on the ethical aspects of DL in hydrology [3]), and it is expected that as the future of hydrology is increasingly connected to the provision of solutions to society's water-related problems, the need to generate reliable solutions in a context in which many of them will be generated by AI/ML/DL, especially those linked to high-stakes decision-making, will be more pressing [8,47,89,102].

The reasons for a greater incorporation of XAI/iML into hydrological research, acknowledging the gaps mentioned in the Introduction section, cannot be separated from the advantages and limitations that these techniques possess. Thus, for example, the most recognized advantage of XAI/iML is its ability to untangle how AI/ML/DL black-box models make their predictions [91], that is, make a model interpretable. In this sense, a model is interpretable if it gives rise to not only mechanistic understanding (transparency) but also to a functional understanding [63]. Regarding the limitations of XAI/iML, some authors mention, for example, that XAI techniques cannot explain events that never happened in the past. "When faced with new and unprecedented circumstances, the explanations provided by XAI may not adequately account for these events, leading to potentially inaccurate forecasts" [103]. This could clearly explain the difficulty of obtaining a higher performance, as we found in this study, when the record includes the effects of an unprecedented drought, such as the one currently affecting the study area. Likewise, limitations are mentioned such as the lack of standardization of metrics and technique evaluation frameworks, a large number of taxonomies of very diverse XAI/iML techniques and, sometimes inconsistent among them, a lack of agreed definitions, etc. [63,103]. At the level of specific techniques, advantages and limitations are also recognized. For LIME, for example, while one advantage might be that "LIME's explanations for an ML model's prediction are optimized to be as simple as possible", some disadvantages are that "LIME only remains faithful in its predictions for an ML model on a localized level" or "Despite the best efforts of LIME's developers to simplify the explanations generated by this algorithm, the interpretability of the final results is still mediocre for non-expert users" [104]. The same occurs in the case of SHAP, where one of its advantages is that "As a mathematically enforced concept Shapley values have additional beneficial properties such as consistency and accuracy" while one of its disadvantages would be that "SHAP has been shown to be inconsistent and vulnerable to adversarial attacks despite the mathematical properties of Shapley Values" [104].

Finally, and even though this study aims to contribute to filling in the current knowledge gaps in XAI/iML/Hydro, there are clearly still several aspects that can be developed in future work. Among them is continuing to investigate issues not yet addressed, or the so-called emerging issues (see Figure 1d, in Section 1, Introduction). Among these, the role of XAI/iML in the interpretation of predictive black-box models associated with drought, water quality, lakes or downscaling applications are a few examples. Another relevant aspect mentioned by other authors is related to the so-called Rashomon Effect, "which describes the following phenomenon: for a given dataset there may exist many models with equally good performance but with different solution strategies. The Rashomon Effect has implications for Explainable Machine Learning, especially for the comparability of explanations" [105]. As recognized by a recent XAI/iML/Hydro study on the matter: "[...] while the field of interpretable ML has started to blossom in the recent past, little attention has been directed to this topic." [106]. The findings of our study, as well as the recognized advantages and limitations of XAI/iML, guide future work in this direction.

5. Conclusions

The present study seeks to contribute to addressing the challenge of expanding the use of XAI/iML globally, particularly in the southern hemisphere, where, apart from in Australia, there is a large adoption gap. It examines the challenge of expanding its application to new research topics, and presents the application of XAI/iML to the prediction of snowmelt-driven streamflow in an arid basin in the north-central region of Chile in the southern hemisphere. The work shows that the use of XAI/iML techniques such as variable importance, partial dependence plots, accumulated local effects plots, Shapley values and local interpretable model-agnostic explanations contribute significantly to the interpretation of the black-box prediction models generated with the Random Forest ML technique. At the model level, the hydrometeorological variables in the vicinity of the basin are more important than the climatic variables in streamflow prediction for one and four months ahead.

The findings also show that the models predict the low streamflow values at the monitoring station for the year 2020 in terms of the hydrometeorological variables in the vicinity of the basin associated with low streamflow and precipitation under drought conditions.

Finally, the importance of contributing to the adoption of XAI/iML in the hydrological community is not only justified by the contribution that this discipline can have in the progress of the understanding of hydrological processes, but also by the role it is having regarding accountability in trustworthy AI/ML/DL for high-stakes decision-making systems.

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Appendix A

Plots in panel a were generated after processing 2008 scientific papers obtained from three bibliographic databases (collections) extracted from the Scopus search engine (www.scopus.com) accessed on 16 May 2023 using three keyword combinations (i.e., (a) Machine learning AND hydrolog*, (b) Deep learning AND hydrolog*, and (c) Artificial intelligence AND hydrolog*), with their respective restriction criteria, for the 2003–2022 record period. The search was conducted in titles, keywords, and abstracts. Publication period (2003–2022), document type (articles), language (English), and subject area (environmental sciences, earth and planetary sciences, agricultural and biological sciences, engineering, computer science, mathematics, energy, multidisciplinary, and decision sciences) were used as inclusion criteria (filters). Each result dataset (collection) was downloaded in csv format, incorporating all available download attributes. The three datasets were combined to then remove duplicates and refine the database (delete records with missing data in the Author, Keyword Plus, and DOI fields)

Plots in panels b, c and d were generated with the same search criteria but using the following keyword combinations (explainable artificial intelligence + hydrolog*; Interpretable machine learning + hydrolog*, XAI + hydrolog*, explainable machine learning + hydrolog*).

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