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RESEARCH ARTICLE - HYDROLOGY AND HYDRAULICS

Hybridizing evolutionary algorithms and multiple non-linear regression technique for stream temperature modeling

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Abstract

The present study hybridizes the new-generation evolutionary algorithms and the nonlinear regression technique for stream temperature modeling and compares this approach with conventional gray and black box approaches under natural flow conditions, providing a comprehensive assessment. The nonlinear equation for water temperature modeling was optimized using biogeography-based optimization (BBO) and invasive weed optimization (IWO), simulated annealing algorithm (SA) and particle swarm optimization (PSO). Two black box approaches, a feedforward neural network (FNN) and a long short-term memory (LSTM) network, were also employed for comparison. Additionally, an adaptive neuro-fuzzy inference system (ANFIS) served as a gray box model for river thermal regimes. The models were evaluated based on accuracy, complexity, generality and interpretability. Performance metrics, such as the Nash–Sutcliffe efficiency (NSE), showed that the LSTM model achieved the highest accuracy (NSE = 0.96) but required significant computational resources. In contrast, evolutionary algorithm-based models offered acceptable performance while reducing the computational complexities of LSTM, with all models achieving NSE values above 0.5. Considering interpretability, accuracy and complexity, evolutionary-based nonlinear models are recommended for general applications, such as assessing thermal river habitats. For tasks requiring very high accuracy, the LSTM model is preferred, while ANFIS provides a balanced trade-off between accuracy and interpretability, making it suitable for engineers and ecologists. While all models demonstrate similar generality, this model is developed for a specific location. For other locations, independent models with a similar architecture would need to be developed. Ultimately, the choice of model depends on specific objectives and available resources.

Keywords Thermal regime · River ecosystem · Data-driven models · Evolutionary algorithms · Black box models

Abbreviations

SNTEPM	Stream network temperature model
SSTEMP	Stream segment temperature model
WAIORA	Water allocation impacts on river attributes
LSTM	Long short-term memory
FNN	Feed-forward neural network
ANFIS	Adaptive neuro-fuzzy inference system
BBO	Biogeography-based optimization
IWO	Invasive weed optimization
PSO	Particle swarm optimization
SA	Simulated annealing algorithm

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Introduction

Aquatic habitats in rivers and lakes have faced significant threats in recent years due to rising global temperatures and human activities within river basins, such as pollutant discharge and water abstraction projects. Water temperature is a critical environmental factor that directly impacts the survival of aquatic species within river ecosystems. Research has consistently shown that water temperature plays a pivotal role in shaping various aspects of aquatic life, including the temporal and spatial distribution of species (Morales-Marín et al. 2019). Moreover, changes in water temperature can disrupt fundamental biological activities of aquatic organisms, such as reproduction and feeding (Walberg 2011; Pankhurst and King 2010; Jonsson and Jonsson 2009).

In recent years, concerns regarding the thermal regime of rivers have intensified due to population growth, climate change and the discharge of various pollutants. These issues are anticipated to worsen as climate change impacts escalate (Missaghi et al. 2017). For decades, the importance of understanding and addressing river temperature regimes has been emphasized in the literature due to their profound influence on biological activities within aquatic habitats.

Broadly, two primary approaches are used to model the thermal regime of rivers. The first involves hydrodynamic heat exchange models, which solve heat flux equations along the river's downstream flow. These models have been extensively utilized over the past decades for thermal budget analysis in rivers, incorporating meteorological and hydrological parameters as well as river reaches characteristics (Dugdale et al. 2017). Known models, such as SNTEMP and WAIORA, have been widely applied to aquatic habitat studies (Bartholow 2002; Wilding et al. 2012). However, a major limitation of these models is their reliance on extensive data for catchment-scale applications. Without the necessary inputs or measurements, their practical utility becomes constrained.

Alternatively, statistical models provide another approach, often used in water quality studies. Linear regression models offer a simple means to study river thermal regimes but are generally not recommended due to their inherent limitations. Nonlinear regression models present a more advanced alternative, though their development and application can be challenging due to the complexities of establishing nonlinear relationships and calculating coefficients and powers in nonlinear equations.

Two critical factors influence the application of data-driven models for river thermal regime modeling: first, selecting the key inputs that affect water temperature, which requires hydrological insights, and second, choosing an appropriate model based on factors such as complexity, accuracy and generality. Regression models are frequently used for river temperature modeling (Arismendi et al. 2014), with model complexity often determining its suitability. Several data-driven models have been developed in the literature to simulate river or water temperature, considering different model types and input combinations (Huang et al. 2023; Das et al. 2022; Heddam et al. 2022; Abdi et al. 2021; Qui et al. 2021; Malekian and Kazemzadeh 2016). However, the applicability of using evolutionary algorithms, particularly new-generation algorithms, in stream temperature modeling has not been fully investigated.

There are many excellent examples of the application of predictive models in hydrology and water science (Xu 2022; Zhang et al. 2022; Zhu 2023; Guo 2024; Yin et al. 2023a, 2023b). These studies highlight that nonlinear regression models, functioning as white box models, enable researchers to identify and quantify the influence of different parameters on outcomes. However, developing these models presents significant challenges due to their computational and methodological complexity. In contrast, machine learning models, which operate as black box models, require more effort to analyze input sensitivities. Neural networks, for example, have been widely used in ecohydrology with promising results (Althoff et al. 2021). Nonetheless, due to their black box nature, interpreting their inner workings and understanding how inputs affect outputs can be difficult, which limits secondary analyses. To address these limitations, neuro-fuzzy models have been introduced, integrating fuzzy inference systems with neural networks. These gray box models offer improved interpretability compared to traditional black box methods (Guerra et al. 2022). However, their interpretability remains somewhat limited when compared to white box models. In this study, the term "gray box" is used to describe these models, acknowledging their intermediate position in terms of interpretability.

A key challenge in river thermal regime modeling is developing robust methods that balance accuracy, interpretability and computational efficiency. This study introduces several novel approaches to advance the field. It presents a nonlinear regression modeling architecture for river thermal regimes, employing biogeography-based optimization (BBO) and invasive weed optimization (IWO), which enhance the capabilities of white box models. These evolutionary algorithm-based models represent a significant innovation, offering strong performance with reduced computational complexity compared to more resource-intensive methods.

Additionally, the study develops black box models, including feedforward neural networks (FNN) and long short-term memory networks (LSTM), as well as a gray box model based on an adaptive neuro-fuzzy inference system (ANFIS). These models showcase advanced techniques for simulating river thermal regimes under natural flow conditions. The incorporation of cutting-edge evolutionary algorithms into white box modeling and the adaptation of neural networks and ANFIS architectures to this domain underline the study's contribution to expanding modeling methodologies.

By emphasizing these innovative modeling approaches, this research provides a transformative framework for addressing the complexities of river thermal regimes, equipping practitioners with tools that align with diverse project objectives and resource constraints.

Application and methodology

Selection of inputs

The selection of model inputs based on simulation data of the river regime is one of the initial steps in developing a robust framework for analyzing the river thermal regime. In this study, a primary hydrodynamic modeling was employed to assess the sensitivity of various inputs in the study area presented in Table 1. It is evident from the analysis that among all influencing parameters, three exhibit notably high sensitivity, potentially significantly impacting the outcomes of thermal modeling. These critical parameters are air temperature, river flow and solar exposure. Consequently, these three factors were chosen as inputs for all models in the study to facilitate a comprehensive comparative analysis across different model types.

Nonlinear regression model (white box)

Drawing upon previous studies and empirical testing, a nonlinear equation was formulated for modeling water temperature. This equation necessitates the calculation or estimation of several coefficients and exponents to establish a dependable model suitable for simulation. Various evolutionary algorithms have been proposed in the literature for developing such nonlinear models of river water temperature simulation. A plethora of evolutionary algorithms exists, encompassing both classic and new-generation approaches (Dokeroglu et al. 2019; Jahandideh-Tehrani et al 2019). In this study, a selection of well-established classic and new-generation evolutionary algorithms was employed, as delineated in Table 2. Moreover, Eq. 1 shows the general form of the nonlinear equation to predict thermal regime of the river flow.

Table 1 Initial sensitivity analysis through heat exchange modeling for selecting inputs

Variable	Relative sensitivity	Selected inputs for data-driven model
River flow	High	*
Inflow temperature	Medium	
Accretion temperature	Low	
Wetted perimeter	Low	
Air temperature	Very high	*
Relative humidity	Medium	
Wind speed	Low	
Ground temperature	Low	
Thermal gradient	Low	
Solar exposure	High	*
Dust coefficient	Low	
Ground reflectivity	Low	
Segment azimuth	Low	
Topographic altitude	Low	
Vegetation height	Low	
Vegetation crown	Low	
Vegetation offset	Low	
Vegetation density	Low	

$$\mathrm{TW} = \left(X1.E^{X2}\right).\left(X3.F^{X4}\right).\left(X5.TA^{X6}\right), \tag{1}$$

where E, F and TA are solar exposure (MJ/m^2), river flow (m^3/s) and TA is air temperature (^{oC}) and TW is water temperature (^{oC}). $X1$ to $X6$ are the unknown coefficients and powers which will be found by the optimization algorithms. The key features of the evolutionary algorithms are mentioned in Table 3.

FNN and LSTM (black box)

In the present study, two black box-based structures were employed to simulate the thermal regime of the river. The first structure utilized a feedforward neural network (FNN), a commonly employed tool in previous hydrological research. Figure 1 illustrates the architecture of this model, featuring three input parameters in the first layer as described, with the output being water temperature. Determining the optimal number of hidden layers is a crucial aspect of this structure. In this study, the number of hidden layers was determined through a separate optimization process. This involved testing various model architectures by adjusting the number of hidden layers and ultimately selecting the configuration with the lowest mean square error. In other words, the best number of hidden layers was identified based on model performance. Moreover, the Levenberg–Marquardt algorithm was applied in the training process of the model.

Optimized number of hidden layer (through assessing root-mean-square error) = 23 layers.

Recurrent neural networks (RNNs) are a type of deep learning model used for predicting or simulating sequential data, such as time series, where both inputs and outputs are sequential. Long short-term memory (LSTM) networks are a variant of recurrent neural networks specifically designed to mitigate the vanishing gradient problem encountered in traditional RNNs. One notable application of LSTMs is time series forecasting, making them highly suitable for a variety of simulations in hydrology and environmental engineering. LSTMs are particularly attractive when there are long-term dependencies between parameters. Detailed discussions on the theory and structure of LSTM networks can be found in existing literature (Le et al. 2019).

Therefore, LSTM should be considered as a viable option for simulating water temperature fluctuations. Water temperature, along with other water quality parameters, is influenced by seasonal changes, indicating that LSTM networks can effectively capture these long-term dependencies to accurately predict water temperature in future time steps. While the inputs remain consistent with other models, the neural network structure is adapted to implement an LSTM model. Recent literature has also explored the use of LSTMs in water quality applications, providing comprehensive insights into the structure of each cell in

Table 2 Selected evolutionary algorithms in this study

Algorithm	Short description	Advantages/ disadvantages	Reference
Biogeography-based optimization (BBO)	Motivated by speciation (the evolution of new species), the migration of species (animals, fish, birds or insects) between islands and the extinction of species	Reasonable computational time for each iteration, lack of guarantee for global optimization, use of habitat suitability index as a robust fitness parameter and limited applications across different fields	(Sedighkia and Datta 2023)
Invasive weed optimization (IWO)	Inspired by the natural behavior of weeds in colonizing	A simple but efficient algorithm, robust for noisy and irregular functions. Reasonable computational time for each iteration, lack of guarantee for global optimization	(Azizipour et.al 2016), (Asgari et.al 2016),
Particle swarm optimization (PSO)	Inspired by swarm's intelligent of the organisms such as bird flock and fish school	Higher computational time compared to BBO and IWO, unsuitable for noisy functions, some other features are similar to IWO and BBO	(Marini and Walczak 2015)
Simulated annealing algorithm (SA)	The name of the algorithm comes from annealing in metallurgy. A probabilistic technique for approximating the global optimum of a given function	Very suitable for very complex noisy and dynamic functions, very high computational time, some other features are similar to other used algorithms	(Bandyopadhyay et al 2008), (Simon 2008)

the network (Pang et al. 2024). Consequently, due to the similarity in the proposed networks and considerable space required for presenting the details, additional details have not been included to streamline the manuscript.

ANFIS (gray box)

In order to enhance the performance and improve the interpretability of modeling, artificial neural networks have been integrated with fuzzy inference systems, resulting in neuro-fuzzy systems. The adaptive neuro-fuzzy inference system (ANFIS) stands out as one of the most popular neuro-fuzzy systems, extensively utilized in environmental and hydrological and water quality studies (Awan and Bae 2014; Kabolizadeh et al 2022). In this data-driven model, a fuzzy inference system is embedded within the structure of a neural network, operating through fuzzy rules to generate outputs. Essentially, a computational map is created to predict outputs in scenarios involving unobserved combinations of inputs. The primary advantage of this system lies in its enhanced interpretability compared to conventional neural networks, which often function as black boxes. Consequently, in this research, this system is referred to as a "gray box." This term reflects the fact that while ANFIS offers greater interpretability compared to black box models, it falls short of the transparency provided by white box models, primarily because it does not produce regression equations like white box systems do, due to its reliance on fuzzy rules and observations. Nevertheless, ANFIS allows for some degree of interpretation regarding the relationship between inputs and outputs. Figure 2 shows the architecture used in the present study. More details of the theory and application of ANFIS-based models have been addressed in the literature (Vargas et al. 2023). We applied hybrid method (backpropagation + least square) to train the ANFIS-based model.

Evaluation indices

Evaluation and measurement indicators are essential for comparing the performance of different models. In this research, we utilized four indicators, developed in numerous past studies, to evaluate the performance of the models. These indicators are all listed in Table 4. Moreover, computational time (minutes) for the training process of each model as well as required memory (CPU usage %) was applied to assess the complexities of the models. More details on the evaluation indices have been addressed in the literature (Yilmaz and Onoz 2020; Gupta et al. 2009).

Table 3 Key features of evolutionary algorithms (EA) in this study

Feature	Description
Objective function	Root-mean-square error (RMSE) between observed time series of river temperature and simulated time series of river temperature by the nonlinear model
Purpose of EA	Minimize the objective function while optimizing coefficient and exponent of three parameter in the Eq. 1
Stopping criterion	The number of iteration (very high number of iteration was considered equal to 10,000)
Initial population	50

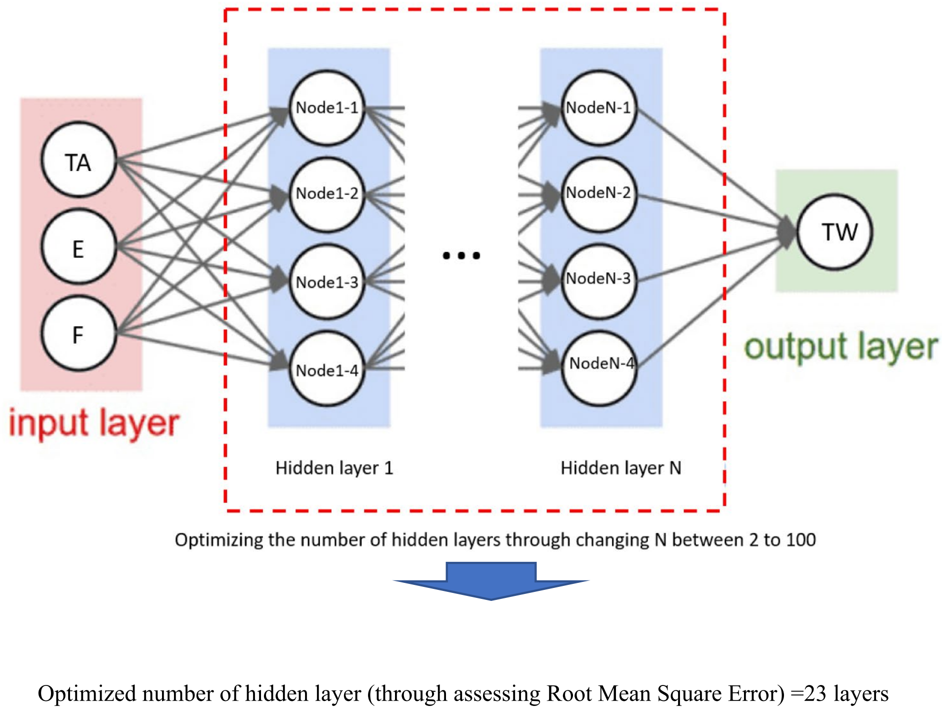


Fig. 1 Proposed architecture of FNN for simulating river thermal regime

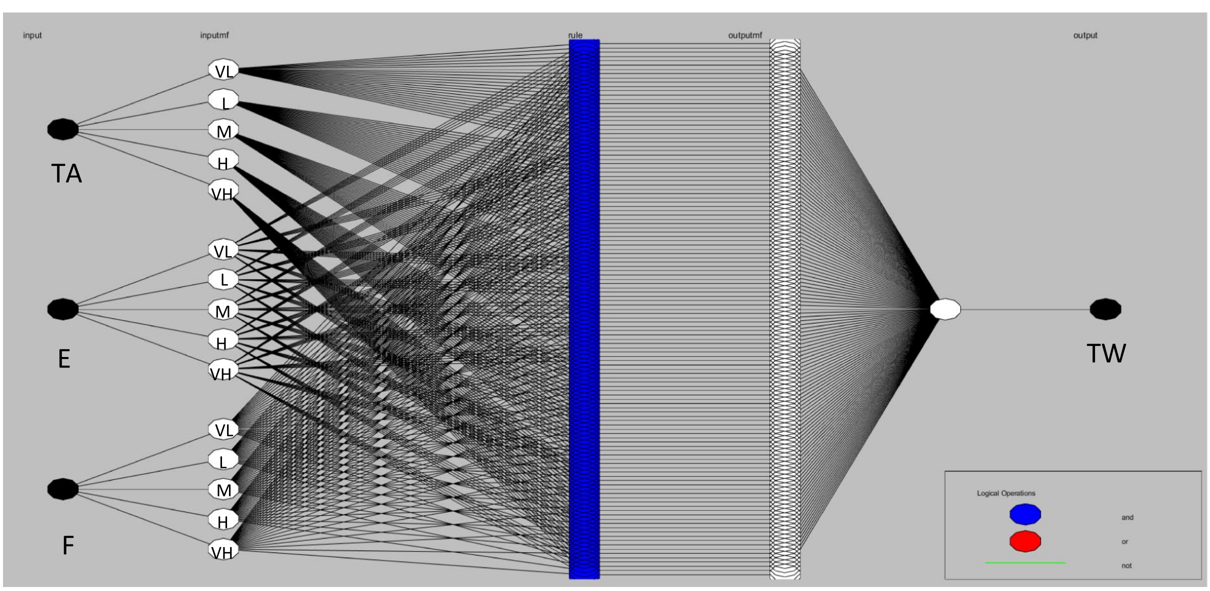


Fig. 2 Proposed architecture of ANFIS for simulating river thermal regime

Table 4 Evaluation indices used in the present study

Index	Mathematical definition	Performance			
		Excellent	Good	Satisfactory	Unsatisfactory
NSE	$\text{NSE} = 1 - \frac{\sum_{t=1}^{T}(\text{OBS}_t - \text{SIM}_t)^2}{\sum_{t=1}^{T}(\text{OBS}_t - \text{OBSm})^2}$	0.75–1	0.65–0.75	0.5–0.65	< 0.5
RSR	$\text{RSR} = \frac{\sqrt{\sum_{t=1}^{T}(\text{OBS}_t - \text{SIM}_t)^2}}{\sqrt{\sum_{t=1}^{T}(\text{OBS}_t - \text{OBSm})^2}}$	0–0.5	0.5–0.6	0.6–0.7	> 0.7
PBIAS	$\text{PBIAS} = 100 * \left(\frac{\sum_{t=1}^{T}(\text{OBS}_t - \text{SIM}_t)}{\sum_{t=1}^{T}(\text{OBS}_t)}\right)$	< ± 10	± 10– ± 15	± 15– ± 25	> ± 25
RMSE	$\text{RMSE} = \frac{\sqrt{\sum_{t=1}^{T}(\text{OBS}_t - \text{SIM}_t)^2}}{\sqrt{T}}$	No specific threshold			

Case study

The Hunter River is a major river in New South Wales, Australia, originating from upstream mountains (1397 m), flowing through the Hunter Valley, and out to sea. Several native aquatic species inhabit this river, which are sensitive to its thermal regime, making environmental protection crucial. Water temperature is a key environmental parameter that must be within suitable ranges to implement optimal strategies for protecting the river ecosystem. The selected study area, depicted in Fig. 3, focuses on an upstream area of the river. Along the river, multiple monitoring stations are established to record water flow, water temperature, and other quality parameters based on available data in the studied area. Our attention is directed toward a key data-recording station where river flow and all significant meteorological parameters have been recorded for a long-term period. The key features of the case study are mentioned in Table 5.

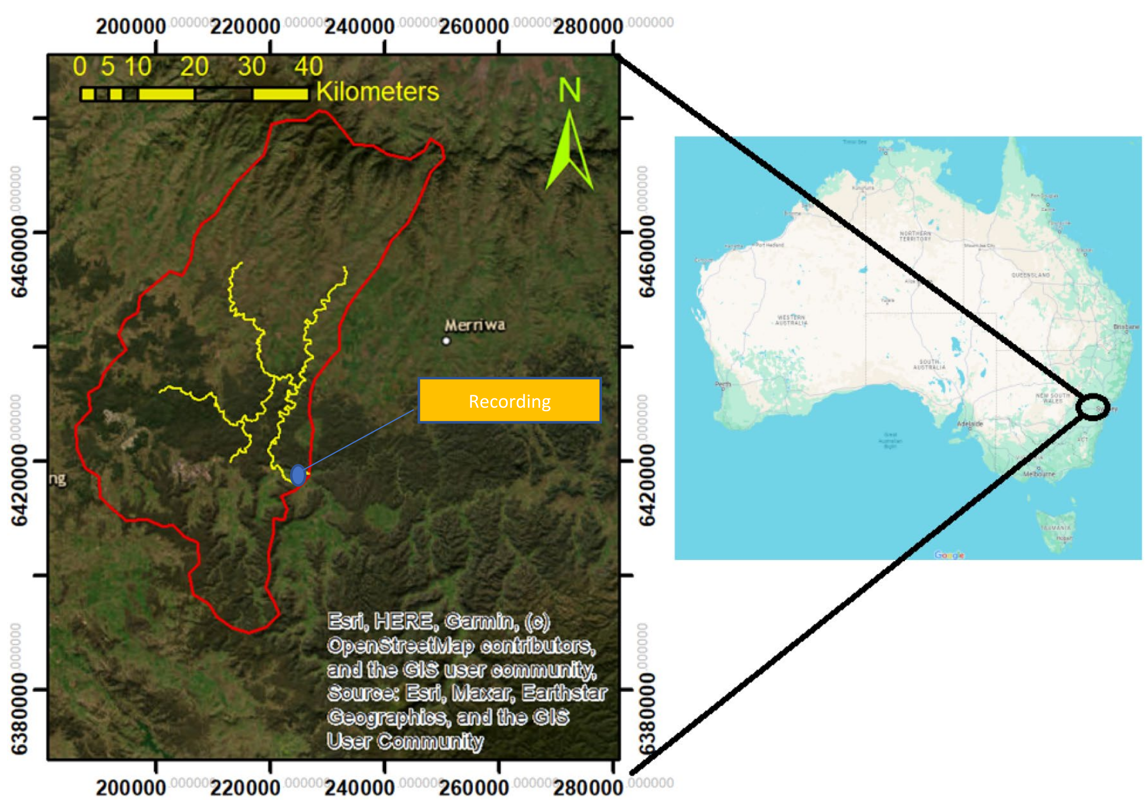


Fig. 3 Location of the case study (redline is the boundary of the sub-catchment, the yellow line is river network in the selected sub-catchment, the blue circle is recording stations used for developed thermal regime models)

Results and discussion

Overview on the modeling results

Figure 4 illustrates the outcomes of simulating the river's thermal regime using a nonlinear model via evolutionary algorithms, juxtaposed with observed river data. From observations, it appears that various evolutionary algorithms demonstrate relatively comparable performance in simulating the river's thermal regime. However, collectively, the fidelity of these models to recorded river data appears somewhat weak, as notable deviations are observed at certain time steps in the simulation compared to the recorded data. Nonetheless, it is important to acknowledge that observational assessment may not be entirely accurate, and metrics for measurement should be employed to gauge accuracy and other facets of its calculations for expert evaluation. Table 6 presents the coefficients and powers of the nonlinear regression models generated through different evolutionary algorithms.

Figure 5 depicts the outcomes of modeling the thermal regime of the river using black box models, notably showcasing higher accuracy, especially with the LSTM model displaying close alignment with observational data. In the subsequent section, various model results are quantitatively compared and evaluated. Figure 6 illustrates the results of river regime modeling utilizing the gray box model, revealing its superior robustness compared to white box models, with a greater resemblance between observational and modeled data. Thus, it is essential to thoroughly analyze and assess these model types in terms of their computational and technical aspects to provide readers with a useful comparison.

Accuracy

As outlined in the preceding section, various measurement indices were employed to assess the accuracy of the models, with the results summarized in Table 7. Upon comprehensive evaluation of these indices, it becomes apparent that the LSM model exhibits superior accuracy compared to other models. However, it is noteworthy that the accuracy of other models is also deemed acceptable, considering the thresholds set by different indices. For instance, based on prior research, an NSE exceeding 0.75 generally indicates excellent model performance, a criterion met by all developed models in this study. This suggests that these models possess acceptable accuracy levels, with high accuracy demonstrated by models like LSTM, underscoring their reliability. In contrast, NSE values for white box models fall between 0.7 and 0.9, indicating the use of a nonlinear model developed through evolutionary algorithms, thereby suggesting acceptable accuracy for these models as well.

The RMSE (root-mean-square error) represents the average squared deviation of model predictions from observed values and serves as a crucial indicator of modeling accuracy. In the evaluation of thermal regime modeling using different approaches, it was observed that the maximum RMSE, approximately 3 °C, was obtained with the nonlinear PSO model, whereas the minimum RMSE, achieved by the LSTM model, was less than half that of the white box models. These variations in RMSE demonstrate that the data-driven models developed in this study can reliably simulate river temperature with satisfactory accuracy.

It is important to note that the acceptable accuracy of a model often depends on its intended application. For example, in studies analyzing water temperature changes in aquatic habitats, an RMSE of 3 °C may be considered negligible, as it falls within the tolerable range of temperature fluctuations for aquatic species. Conversely, for applications requiring precise temperature predictions, the LSTM model is recommended as a black box solution, as it achieves

Table 5 Key features of the case study

Feature	Description
Catchment area	~21,500 km^2 (largest coastal catchment in NSW)
River length	~460 km (flows from the Barrington Tops to Newcastle)
Major tributaries	Goulburn, Paterson, Williams, Wollombi, Pages, Isis Rivers
Hydrological and meteorological data availability	Long-term data (40 years) are available. However, data gaps before 2011 are considerable
Climate	Highly variable, prone to droughts and floods
Thermal regimes	Considerable difference between minimum and maximum water temperature in each year
Range of data for thermal modeling	Continuous available thermal data between 2012 and 2020
Scale of modeling	Daily scale thermal model
Training data	80% of available data for training (approximately between 2012 and 2018)
Training data	20% of available data for training (approximately between 2018 and 2020)

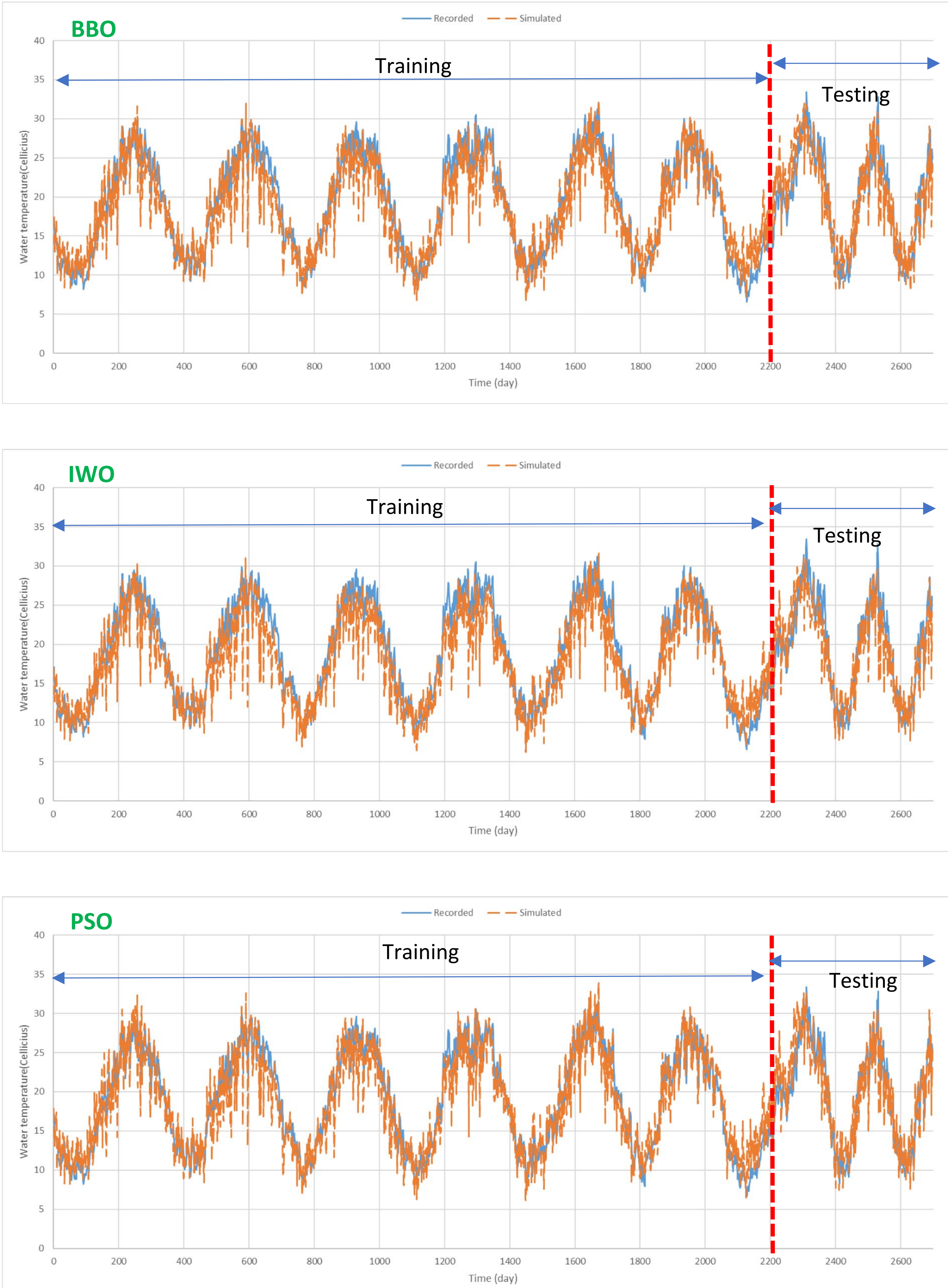


Fig. 4 Results of thermal regime modeling by the white box models

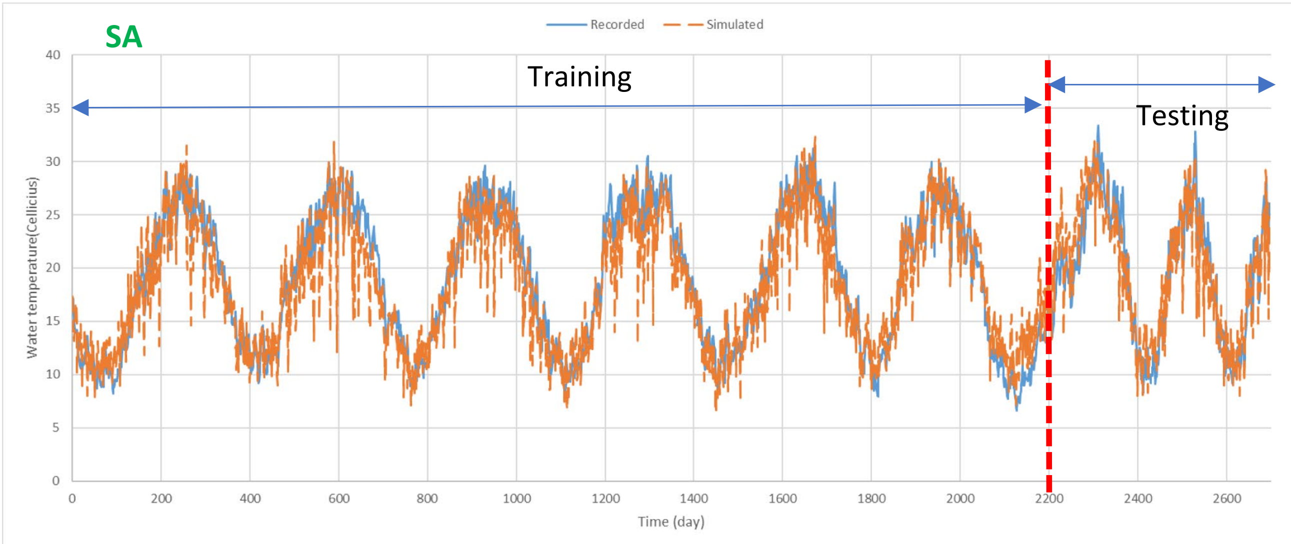


Fig. 4 (continued)

Table 6 Constant coefficients and powers of the white box models

Algorithm	X1	X2	X3	X4	X5	X6
BBO	3.141947	0.1563	−4.09892	0.003076	−0.14302	0.66336
IWO	9.884344	0.187977	0.034899	0.008942	4.735997	0.65498
PSO	−2.41735	0.147399	−0.13116	0.018807	4.661408	0.733503
SA	0.548406	0.203593	1.242998	0.007068	2.469186	0.640026

an RMSE of less than 1.5 °C, reflecting its high accuracy. Moreover, a comparison of other performance indicators and observational data with simulation outputs reveals that the LSTM model successfully simulates local maximum and minimum water temperature values with notable precision, making it a reliable tool for modeling the full time series of water temperature extremes.

The demonstrated accuracy of white, gray and black box models, particularly the LSTM as the most accurate, highlights that considering just three key parameters is sufficient to achieve highly reliable results when modeling river thermal regimes. This finding underscores that there is no need for complex heat exchange models for station-scale simulations, as such approaches often complicate data acquisition and the modeling process without significantly improving results. Thus, accurate data-driven models offer a practical and efficient alternative.

Another noteworthy result is the high accuracy of nonlinear models in simulating river thermal regimes. This study indicates that nonlinear models, particularly those utilizing evolutionary algorithms to optimize variable parameters, can effectively function as white box models capable of accurately simulating the thermal regime of rivers. Consequently, employing evolutionary algorithms to develop suitable nonlinear regression models is strongly recommended for applications requiring interpretable and precise modeling frameworks.

Figure 7 shows Taylor diagram of different data-driven models. The x-axis indicates the ratio of the model's standard deviation to that of the observed data. A value closer to 1 indicates that the model captures the variability of the observed data well. The angular position of a point reflects the correlation between the model output and the observed data. Higher correlation values (closer to the observed point) indicate better performance. The radial distance from the observed point indicates the RMSE. A shorter distance implies better model performance. LSTM stands out as the best-performing model, excelling in all three metrics: standard deviation ratio, correlation coefficient and RMSE. This highlights its suitability for accurately modeling river thermal regimes, while computational complexity might be questionable. ANFIS and FNN are practical choices when computational resources are limited. IWO, BBO and SA underperform compared to the others, with lower correlation coefficients and higher RMSE values. However, these models are still acceptable in terms of accuracy and they may be simpler and computationally efficient.

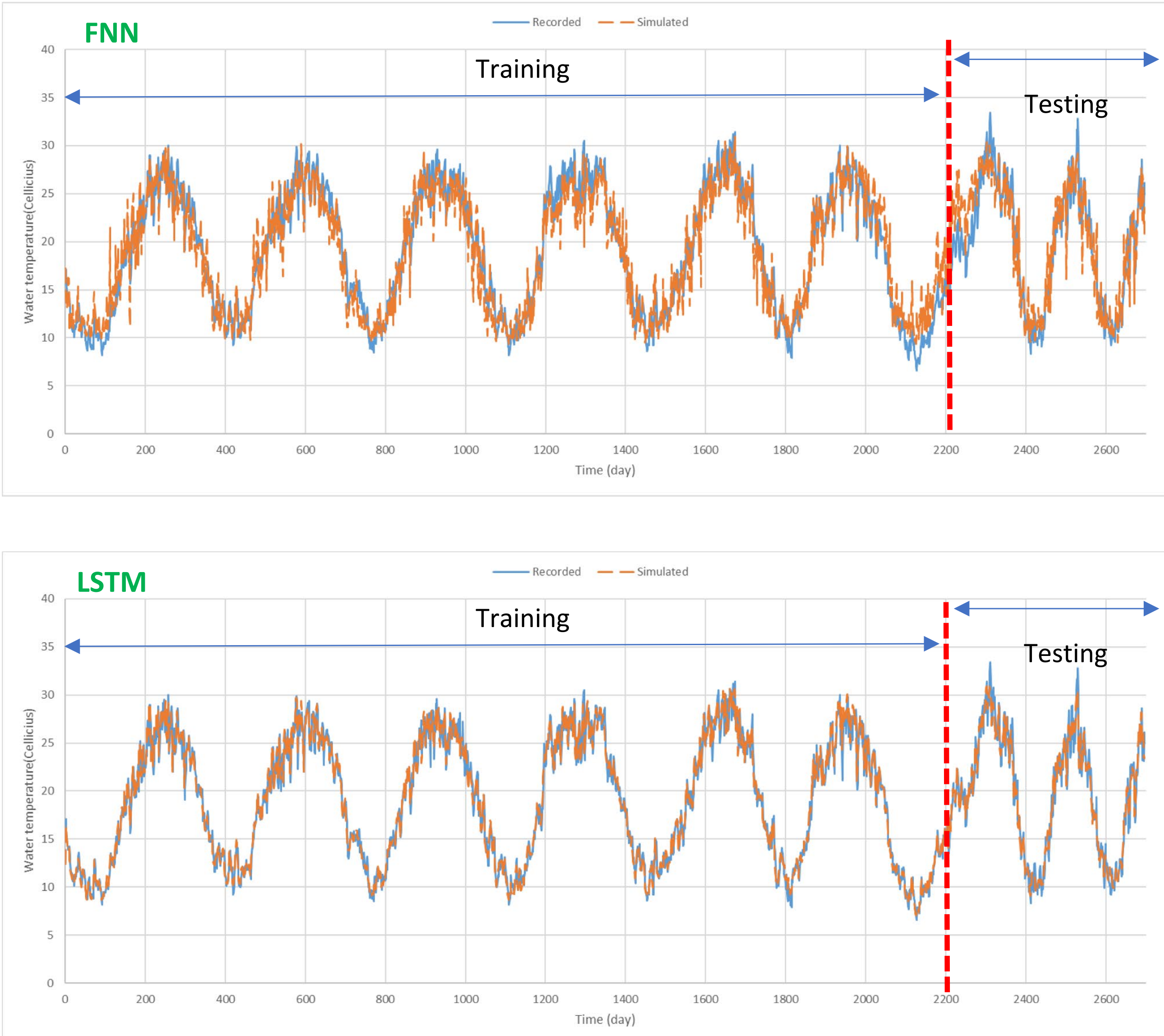


Fig. 5 Results of thermal regime modeling by the black box models

Complexities

The computational complexity of a model is a critical criterion for selecting the most suitable model in a project, as high complexity can hinder the model's usability. Generally, engineers, who are the end-users of data-driven models, prefer simpler and less complex models for their studies. As defined in previous studies, the computational complexity of a model refers to the time and memory required to obtain the best solution, which can vary significantly depending on the model type, number of input parameters and the proposed architecture. In this study, two parameters were considered to evaluate the computational complexity of the thermal regime model including 1) the computing time for model training and 2) the memory required during model training. For all proposed architectures, the number of iterations was set to 5000. Based on conducted tests, it was determined that 5000 iterations lead to acceptable convergence, as observed during models' development in this case. Notably, in the development of white box models, the number of iterations represents the number of iterations of the evolutionary algorithm needed to achieve the optimal coefficients and powers for the nonlinear model. In black box and gray box models, this number of iterations is used to train the model and determine the optimal coefficients in the neural network. Table 8 presents the computing time and required memory for all types of models. It is evident that the LSTM model demands a substantial amount of computing time compared to other

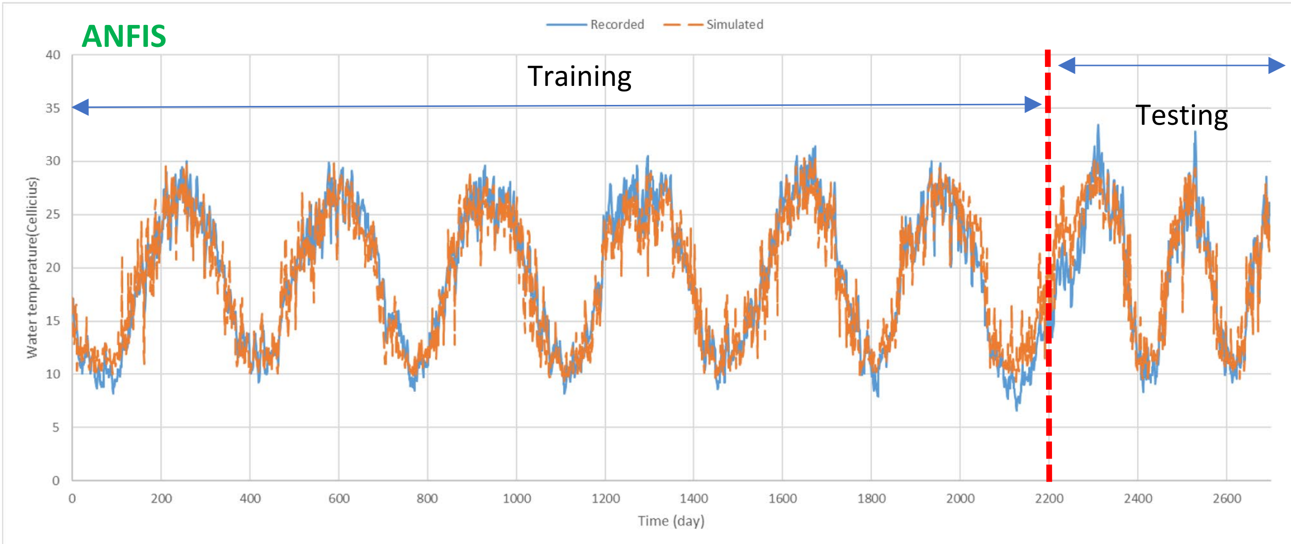


Fig. 6 Results of thermal regime modeling by the gray box model

Table 7 Evaluation indices of different modeling frameworks in this study

Index	White box models				Gray box model	Black box models	
	BBO	IWO	PSO	SA	ANFIS	FNN	LSTM
NSE	0.78	0.77	0.77	0.76	0.82	0.81	0.96
RSR	0.21	0.22	0.22	0.23	0.18	0.18	0.035
PBIAS	−2.5	1.03	−2.4	−1.75	−4.17	−3.88	0.086
RMSE	2.9	2.95	2.94	3	2.63	2.64	1.17

models. However, the computing time for other models is relatively similar, with no significant difference observed among them except SA-nonlinear regression which needed more time compared to other evolutionary algorithms. Therefore, all models except LSTM might be considered similar in terms of computational time. Regarding memory usage during the training period, the LSTM black box model necessitates more memory (CPU usage %) during simulation compared to other architectures. Conversely, the discrepancy in memory requirements between other models is insignificant. It should be noted that developing a white box model through evolutionary optimization somehow needs the same time and memory with the FNN and ANFIS-based models.

Generality and interpretability

All developed models demonstrate the same level of generality, indicating that they can be equally applied across various cases. This consistency highlights the importance of the three key parameters influencing river water flow in this study, as they are likely to impact the thermal regime of rivers in other scenarios as well. Several types of nonlinear functions can be developed to predict the thermal regime of rivers. In this study, a specialized nonlinear function was formulated with several notable advantages. First, this function was designed based on key parameters influencing river water temperature, primarily recorded at meteorological stations, making the required data widely accessible. This accessibility enhances the practicality of the function for widespread applications. Additionally, the nonlinear function was intentionally developed to facilitate straightforward modeling for engineers.

Preliminary hydrodynamic modeling revealed that river water temperature is highly sensitive to these three parameters, indicating their significant influence. The nonlinear function presented in this research incorporates coefficients and exponents for each parameter, enabling effective modeling of environmental variables like river water temperature. This dual consideration of coefficients and powers ensures the flexibility needed to optimize these values based on the available data and the unique ecological and hydrological characteristics of the studied river. Consequently, the proposed model can address both data accessibility and robustness of water temperature models, making it highly adaptable to different applications. While the developed models and their architectures are broadly applicable, future

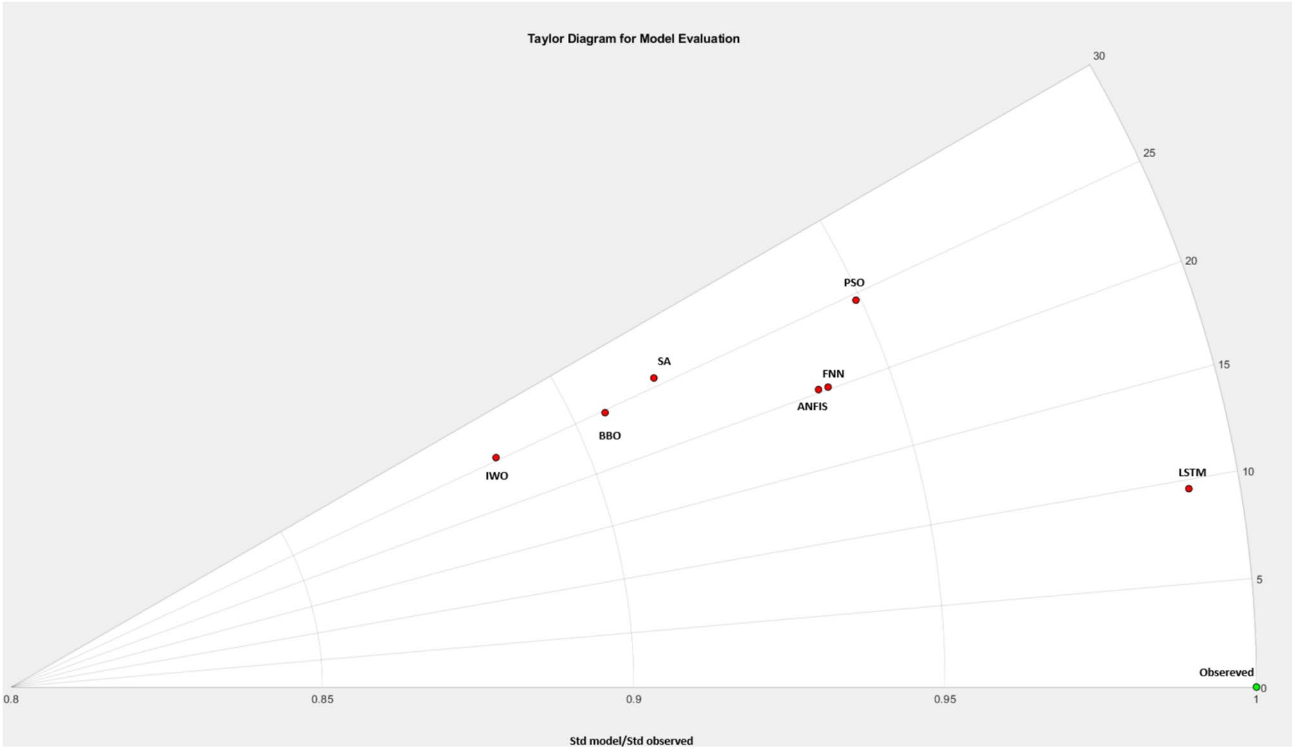


Fig. 7 Taylor diagram for different data-driven models

Table 8 Computational complexities of different models

Type of model	Computational time for training the model (minutes)	CPU usage(%) during the training process
White box model (BBO-nonlinear regression)	178	42%
White box model (IWO-nonlinear regression)	192	42%
White box model (PSO-nonlinear regression)	175	42%
White box model (SA-nonlinear regression)	321	44%
Black box model (FNN)	185	41%
Black box model (LSTM)	651	61%
Gray box model (ANFIS)	189	43%

research can focus on incorporating additional parameters to enhance predictive accuracy for specific case studies or tailored applications.

A major distinction among the models lies in their interpretability concerning the river's thermal regime. White box models offer high interpretability, making it possible to conduct detailed analyses of the influence of input variables on the thermal regime. This characteristic makes white box models particularly valuable for ecologists, as they enable a clear understanding of the effects of key parameters such as air temperature and river flow. On the other hand, black box models, such as the LSTM network, excel in simulating the temperature regime with high accuracy but are less favored for interpretive tasks due to their opaque nature. While black box models may outperform white box models in terms of predictive accuracy, the high interpretability of white box models remains a significant advantage.

The choice between these modeling approaches largely depends on the project's objectives. If the primary goal is precise prediction, black box models are the preferred choice. Conversely, if the aim is to interpret the effects of input parameters on the thermal regime, white box models are more suitable.

The results of this study indicate that air temperature has the most significant impact on the thermal regime of rivers compared to the other two parameters. Solar radiation exposure also plays an important role, though its effect is somewhat secondary, while the influence of river flow rate is comparatively less pronounced. Interestingly, the performance of different evolutionary algorithms showed no substantial variation in determining the impact of input parameters on the thermal regime of river flow.

Gray box models offer an intermediate level of interpretability, bridging the gap between white and black box models. While not as interpretable as white box models, gray models are more transparent than black box approaches. For example, the ANFIS model provides some degree of interpretability through its fuzzy rule system. As illustrated in Fig. 8, these fuzzy rules contribute to understanding the thermal regime but still fall short of the clarity provided by white box models.

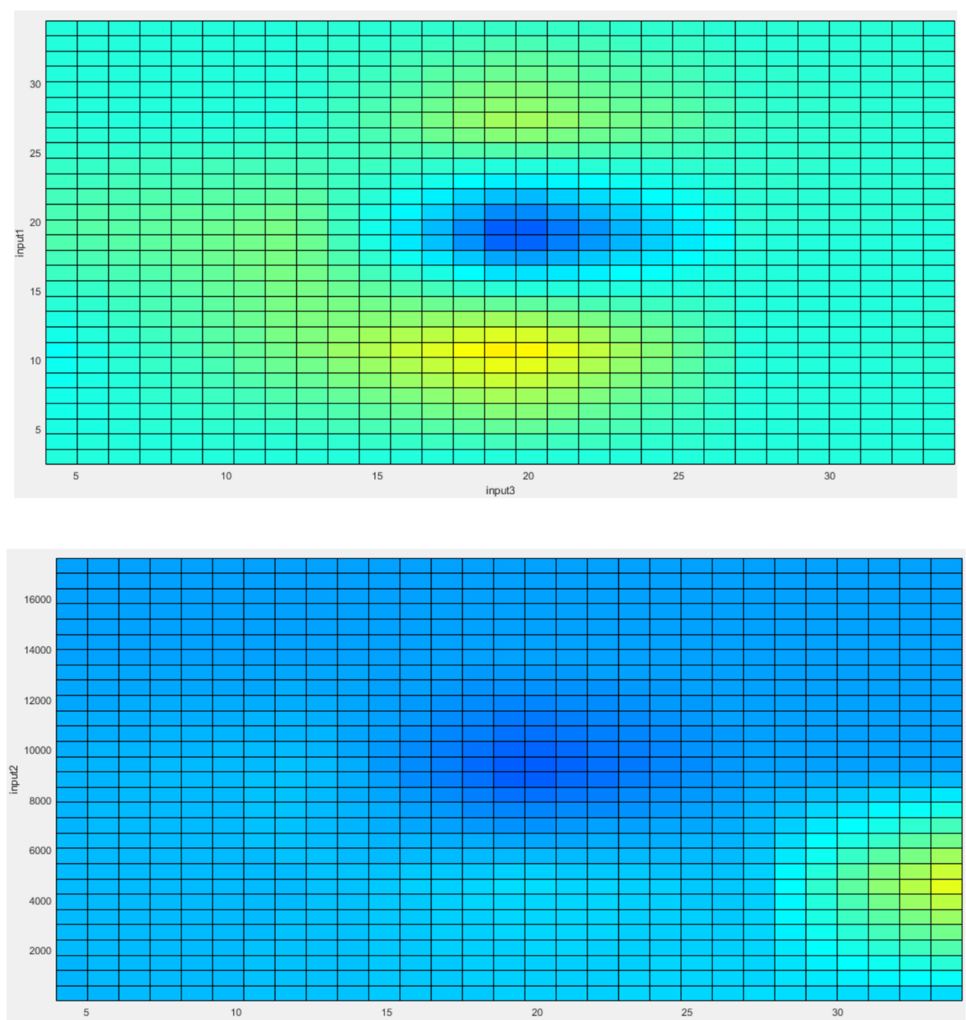
For projects where both interpretability and predictive accuracy are desired, gray box models serve as a balanced alternative. They are particularly well-suited for ecologists working on river thermal modeling projects, offering greater interpretability than black box models while achieving higher accuracy than white box approaches.

Limitations

Each mathematical model has inherent limitations that should be carefully considered when applying the described methods. Readers of this research are encouraged to take these constraints into account to ensure appropriate usage. The primary limitation of all models developed in this study is the restricted number of input parameters. We have only tested one combination of the inputs in this study. However, more combination of inputs can be tested for any potential improvement.

Another notable limitation of the proposed thermal regime model is its applicability being confined to specific river locations. The models were developed using data from a single hydrometric station, which restricts their generalizability to other sections of the river. To achieve a comprehensive understanding of the thermal regime at a catchment scale, separate models must be developed for key hydrometric stations along the river. In other words, in this case, the model is developed based on data from a specific location

Fig. 8 Pseudo-color graphs for interpretability of results of ANFIS-based model (input1, input2 and input3 are solar exposure, river flow and air temperature, respectively)



along the river. In other words, it is capable of simulating water temperature at this particular location but cannot be directly applied to other locations along the river. This represents a limitation of the current model. For other locations, independent models with a similar architecture would need to be developed. However, this approach can significantly increase project costs and may become financially prohibitive.

For projects seeking to model the thermal regime at the catchment scale, it is recommended to integrate hydrodynamic heat exchange models with the approaches proposed in this study. On the other hand, for projects focused on assessing the thermal regime's impact on aquatic environments within specific key river habitats, the use of complex heat exchange models may not be necessary. In such cases, the modeling architecture proposed in this study provides an efficient and accurate solution tailored to this specific application.

Advances compared to the literature and future research directions

The alterations in river thermal regimes hold significant importance in the study of riverine aquatic ecosystems. Various biological activities of organisms are influenced by the thermal regime, as observed in prior studies that primarily examined the effects of water temperature through field observations or modeling approaches. However, hydrodynamic models exhibit a significant limitation in simulating water temperature time series due to their inflexibility in accommodating diverse scenarios. For example, the SNTEMP/SSTEMP models, widely recognized for simulating river thermal regimes in fish habitats, such as those of Brown trout (Sedighkia et al. 2019), require a complete model setup for each new scenario. This process depends heavily on the availability of accurate input parameters, which may not always be feasible across various study areas and scenarios.

In contrast, the architecture proposed in this study overcomes these limitations. By establishing relationships between three key input parameters, it enables the simulation of numerous unobserved scenarios. Inputs for such scenarios can be inferred based on the identified relationships, offering a more adaptable approach. While some studies have utilized data-driven models to analyze river thermal regimes, this study marks significant progress by conducting a comprehensive comparative analysis of thermal regime modeling approaches. These comparisons are vital given the statistical nature of the models, the hydrological characteristics of the study area and the project objectives. The choice of a model for a particular project should align with the objectives set by regional ecologists or water resources engineers.

Although previous studies have demonstrated acceptable accuracy in using data-driven models for river thermal regime simulation (Zhu et al. 2019), they often lack an evaluation of critical factors such as model complexity, interpretability and application limitations. This study highlights the utility of data-driven models for exploring river temperature regimes, addressing gaps in the existing literature.

Future research should focus on incorporating spatial scale into data-driven models to address location-specific limitations. Optimally integrating spatial scale as an input parameter could significantly enhance model performance. The models developed in this study hold the potential to replace hydrodynamic heat exchange models entirely in certain applications. For instance, hydrodynamic heat exchange models are traditionally used to determine environmental flows in rivers, particularly through methodologies such as the instream flow incremental method. However, these models often entail high costs due to their inherent limitations. Adapting the proposed architecture to include spatial scale as an input parameter could streamline the simulation of environmental flow regimes, reducing reliance on costly conventional methods.

Another promising research direction involves extending the proposed architecture to account for the impacts of hydraulic structures, such as large dams, on thermal regimes. Modifying the architecture to incorporate these effects would enable more comprehensive modeling of thermal regimes in future studies (see Di Baldassarre et al.., 2021; Sedighkia et al. 2022).

Concluding remarks

This study introduces a novel architecture for modeling the thermal regime of rivers, utilizing a range of data-driven models, including white box, black box and gray box models. These models were compared through a case study simulation, providing valuable insights into their performance and suitability for different applications.

Among the proposed models, black box models, particularly the long short-term memory (LSTM) network, demonstrated superior accuracy in predicting the river's thermal regime. However, LSTM's higher computational complexity, in terms of training time and memory requirements, limits its practical applicability for large-scale implementations.

In contrast, nonlinear regression models developed through evolutionary optimization, as a white box model, proved to be a robust method for simulating river thermal regimes. These models offer significant advantages in terms of interpretability, making them particularly suitable for applications such as fish habitat analysis where understanding input parameter effects is crucial.

Gray box models, such as the adaptive neuro-fuzzy inference system (ANFIS), not only provided better performance than white box models but also offered an intermediate level of interpretability. This makes them a promising choice for scenarios where a balance between model accuracy and interpretability is desired.

The findings of this study underscore the importance of selecting the appropriate modeling approach based on the specific objectives of the study. A key limitation of the proposed models is the absence of spatial scale as an input parameter, restricting their applicability to site-specific scales. Future research should focus on incorporating spatial scale into the model architecture to enable its application at the watershed scale, enhancing its utility for broader environmental and ecological studies.

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Declarations

Conflict of interest None.

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