



# Extended range forecasting of stream water temperature with deep learning models

Ryan S. Padrón<sup>1,2</sup>, Massimiliano Zappa<sup>1</sup>, Luzi Bernhard<sup>1</sup>, Konrad Bogner<sup>1</sup>

<sup>1</sup>Research Unit Mountain Hydrology and Mass Movements, Swiss Federal Institute for Forest, Snow and Landscape Research WSL, Birmensdorf, Switzerland

<sup>2</sup>Institute for Atmospheric and Climate Science, ETH Zurich, Zurich, Switzerland

Correspondence to: Ryan S. Padrón (ryan.padron@wsl.ch)

**Abstract.** Stream water temperatures influence water quality with effects on aquatic biodiversity, drinking water provision, electricity production, agriculture, and recreation. Therefore, stakeholders would benefit from an operational forecasting service that would support timely action. Deep learning models are well-suited to provide probabilistic forecasts at individual stations of a monitoring network. Here we train and evaluate several state-of-the-art models using 10 years of data from 54 stations across Switzerland. Static catchment features, time of the year, meteorological observations from the past 64 days, and their ensemble forecasts for the following 32 days are included as predictors in the models to estimate daily maximum water temperature over the next 32 days. Results show that the Temporal Fusion Transformer (TFT) model performs best with a Continuous Rank Probability Score (CRPS) of 0.70 °C averaged over all lead times, stations, and 90 forecasts distributed over 1 year. The TFT is followed by the Recurrent Neural Network Encoder – Decoder with a CRPS of 0.74 °C, and the Neural Hierarchical Interpolation for Time Series with a CRPS of 0.75 °C. These deep learning models outperform other simpler models trained at each station: Random Forest (CRPS = 0.80 °C), Multi-layer Perceptron neural network (CRPS = 0.81 °C), and Autoregressive linear model (CRPS = 0.96 °C). The average CRPS of the TFT degrades from 0.38 °C at lead time of 1 day to 0.90 °C at lead time of 32 days, largely driven by the uncertainty of the meteorological ensemble forecasts. In addition, TFT water temperature predictions at new and ungauged stations outperform those from the other models. When analyzing the importance of model inputs, we find a dominant role of observed water temperature and future air temperature, while including precipitation and time of the year further improve predictive skill. Operational probabilistic forecasts of daily maximum water temperature are generated twice per week with our TFT model and are publicly available at <https://www.drought.ch/de/impakt-vorhersagen-malefix/wassertemperatur-prognosen/>. Overall, this study provides insights on the extended range predictability of stream water temperature, and on the applicability of deep learning models in hydrology.

## 1 Introduction

The services provided by streams and rivers are conditioned by water quantity as well as quality (van Vliet et al., 2017, 2023). For water quality, temperature is a key and highly sensitive variable as recognized by scientists, practitioners, and



regulators (e.g. Arora et al., 2016; Hannah et al., 2008; Hannah and Garner, 2015; Johnson et al., 2024; Webb, 1996). Water temperature affects growth, reproduction, distribution, health, and survival of aquatic life (e.g. Alfonso et al., 2021; Booker et al., 2022; Elliott and Elliott, 2010; Hannah and Garner, 2015; Little et al., 2020; Singh et al., 2024), as well as dissolved oxygen (Chapra et al., 2021) and nutrient cycling (Comer-Warner et al., 2019; Johnson et al., 2024). Economic and societal  
35 aspects of electricity production, drinking water provision, recreation, and tourism are also conditioned by water temperature (e.g. Michel et al., 2020; Ouellet et al., 2020; van Vliet et al., 2013). As we undergo the effects of the human-induced climate crisis, more frequent and new challenges related to changes in water temperature are expected (Caretta et al., 2022; Ficklin et al., 2023; Hardenbicker et al., 2017; Michel et al., 2022; van Vliet et al., 2023).

40 Data-informed decisions are essential to adequately address present and future challenges associated to stream water temperature. The ongoing expansion of monitoring networks and water temperature research (Ouellet et al., 2020) are steps in the right direction. Whereas this largely applies to Europe and North America, throughout most of the world water temperature data remain sparse, restricted, and fragmented in space and time (Ficklin et al., 2023; Hannah et al., 2011; van Vliet et al., 2023). In addition, observed and projected long-term stream water temperature regional warming trends (Arora  
45 et al., 2016; Hardenbicker et al., 2017; Kelleher et al., 2021; Michel et al., 2020, 2022) are often insufficient for stakeholders that require timely information from individual streams at high temporal resolution. The monitoring network of the Swiss Federal Office for the Environment aims to satisfy these requirements and is used in this study to predict daily maximum water temperature across a wide range of river stations.

50 Stream temperatures across regions are primarily determined by climate, with air temperatures having a dominant effect. Nevertheless, the relationship between air and water temperature at individual catchments is mediated by the local meteorology, hydrology, and watershed characteristics (Hannah and Garner, 2015; Wade et al., 2023). Typically, air temperature and runoff are used to predict stream temperature (e.g. Qiu et al., 2021; Toffolon and Piccolroaz, 2015; Zhu and Piotrowski, 2020), and less often solar radiation, precipitation, and base flow (groundwater contribution) have also been  
55 considered (Arora et al., 2016; Feigl et al., 2021; Wade et al., 2023). The response of water temperature to changes in these environmental conditions can vary according to catchment characteristics (Wade et al., 2023). In Switzerland, contributions of glacier/snow meltwater are relevant as they reduce the sensitivity of stream temperature to an increase in air temperature (Michel et al., 2020). Another important aspect is the shorter hydrologic residence time of small steep catchments, which hinders their ability to accumulate heat compared to larger flatter catchments that often encompass lakes. Lastly, direct  
60 human impacts from reservoir management, water withdrawal, wastewater discharge, urbanization, etc, further increase the complexity of processes influencing stream temperatures (Ficklin et al., 2023).

Statistical data-driven models are used to predict stream water temperature in an operational setting relevant for decision-making, given that it is usually not possible to meet the high data requirements of process-based models to solve the energy



65 transfer equations to and from the river (Benyahya et al., 2007; Dugdale et al., 2017; Feigl et al., 2021; Zhu and Piotrowski,  
2020). Statistical models estimate water temperature as a function of related covariates and range from simple linear  
(auto)regression models to novel deep learning model architectures (Tripathy and Mishra, 2023). The results from Feigl et al.  
(2021) for 10 river stations in Austria show an average mean absolute error of 0.44 °C for the best performing machine  
learning models out of set including: Random Forest, XGBoost, Feed-Forward neural networks, and Long Short-term  
70 Memory (LSTM) recurrent neural networks. These machine learning models clearly improve the prediction of daily water  
temperature compared to the average mean absolute error of 1.24 °C for linear regression and 0.76 °C for the Air2stream  
hybrid model, which combines a physically based structure with a stochastic calibration of the parameters (Toffolon and  
Piccolroaz, 2015). In another study with data from 8 river stations in the United States, Switzerland and China, Qiu et al.  
(2021) found an average mean absolute error of 0.57 °C for a deep learning LSTM, which outperformed Air2stream, a  
75 Random Forest model, and a Back Propagation neural network. To date there are novel deep-learning architectures with  
promising results for time series forecasting (Challu et al., 2023; Lim et al., 2021; Wen et al., 2018), which are yet to be  
applied to forecasting water temperatures (Tripathy and Mishra, 2023).

Here we evaluate the skill of three of these state-of-the-art deep-learning models for predicting daily maximum water  
80 temperature in 54 river stations in Switzerland over the next 32 days since the start of the forecast against three more  
common and simpler models. An important innovation of these models is direct multi-horizon forecasting (i.e. the  
simultaneous prediction of multiple future time steps) instead of iteratively forecasting one day after another, which  
increases efficiency and robustness (Challu et al., 2023; Fan et al., 2019; Lim et al., 2021). Furthermore, some of these  
models produce probabilistic forecasts that are useful for risk management under uncertainty. We also assess the uncertainty  
85 stemming from the forecasts of meteorological variables that are used as predictors of stream temperature. Counting with  
probabilistic stream temperature forecasts over the upcoming month allows users to optimize the timing of their actions, such  
as adaptation measures when facing extreme conditions (e.g. Ouellet-Proulx et al., 2017). The analysis of extend range  
forecasts is a novel aspect of our study that goes beyond the traditional focus on one-step-ahead forecasts. In this study we  
also analyse the extrapolation capabilities of the deep learning models to predict stream water temperature at new and  
90 ungauged stations, as well as the predictive importance of model inputs and previous time steps. Lastly, we present an  
example of our operational forecasts with the best performing model.

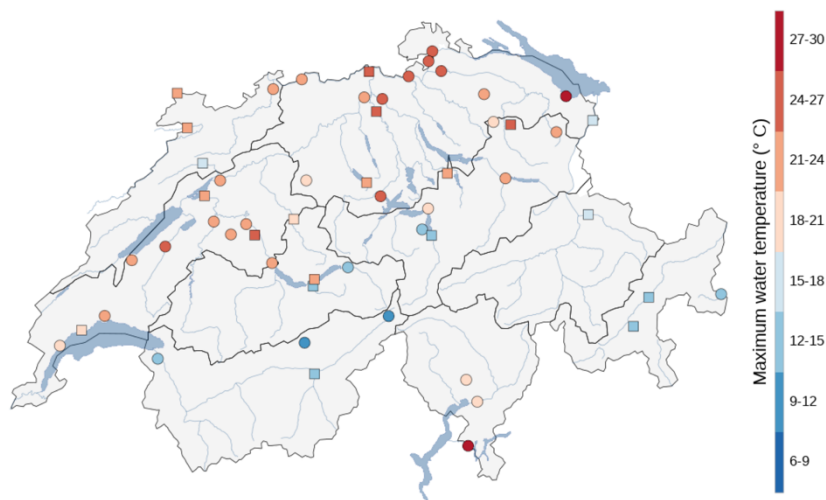
## 2 Methods

### 2.1 Data

We use a subset of 54 stations from the Swiss Federal Office for the Environment monitoring network  
95 (<https://www.hydrodaten.admin.ch/en/>) (Fig. 1 and Table S1). Our variable of interest is daily maximum stream water  
temperature (WT), and for the analysis we use data from 12/05/2012 until 31/12/2022. In addition, we employ



meteorological data, plus information on catchment characteristics and time of the year as relevant features for forecasting stream water temperature.



100 **Figure 1: Map of 54 stream water temperature stations in Switzerland used for the analysis.** The color bar indicates the observed mean annual maximum daily water temperature from 2012 to 2022. Squared markers indicate the subset of stations not used for training the models when evaluating the predictive skill at new and ungauged stations.

The area of the catchments ranges from 3.19 km<sup>2</sup> for station 2414 (Rietholzbach - Mosnang, Rietholz) to 34524 km<sup>2</sup> for station 2091(Rhein - Rheinfelden, Messstation), and the mean elevation from 503 m for station 2415 (Glatt - Rheinsfelden) to 2704 m for station 2256 (Rosegbach - Pontresina). Glacierized area fraction can reach up to 24.7% for station 2269 (Lonza - Blatten). Table S1 details the catchment characteristics from the 54 stations. To inform about the time of the year we define a date index (DI) as a sine function of the week of the year (woy) (Eq. 1), such that values range from near 0 at the end of January (winter) up to 1 at the end of July (summer). A modified date index as a predictor has been shown to improve the skill and/or training time of models (Feigl et al., 2021; Zhu and Piotrowski, 2020).

110

$$DI = \left| \sin \left( \pi * \left( woy - \frac{52}{12} \right) / 52 \right) \right| \quad (1)$$

The considered meteorological variables include daily average near surface air temperature (AT), precipitation (P), and daily fraction of sunshine duration (SD). Gridded data of these variables is provided by the Swiss Federal Office for Meteorology and Climatology at a spatial resolution of 2 km. For simplicity we use for each station the time series of these variables from the single grid cell where the station is located, given the spatial coherence between neighboring grid cells. In addition to past observed values of these meteorological variables, their forecasts for the next 32 days are taken into account to forecast stream water temperature up to the same lead time. The meteorological forecasts correspond to a downscaled version of the Extended-range forecasts from the European Centre for Medium-Range Weather Forecasts (ECMWF), following the setup presented and used by Bogner et al. (2022) and Chang et al. (2023) for streamflow forecasting. We use the ensemble

120



forecasts with 51 members (1 control and 50 perturbed initial conditions) provided by ECMWF to estimate the increasing uncertainty with lead time.

## 2.2 Forecasting models

We use three deep-learning models: Recurrent Neural Network Encoder – Decoder (RNNED), Temporal Fusion Transformer (TFT), and Neural Hierarchical Interpolation for Time Series forecasting (NHITS). In addition, we use three more common and simpler models: Autoregressive linear model with exogenous variables (ARX), Random Forest (RF), and Multi-layer Perceptron neural network (MLP) with one hidden layer to put our results into context with previous studies. Data from 2012 to 2021 is used for training the models, whereas data from 2022 is used for evaluating their predictions. For all deep-learning algorithms a single general model is trained with data from all 54 stations, and daily values for the next 32 days are predicted in a single forward pass. On the other hand, the ARX, RF, and MLP models are trained separately for each station and forecasts are produced iteratively one day at a time up to the 32 days lead time. TFT, NHITS, RF and MLP generate quantile forecasts of q2, q10, q25, q50, q75, q90, and q98; whereas RNNED and ARX predict a single best estimate. Source code and implementations of the deep-learning models we employ are publicly available in the PyTorch Forecasting documentation (Beitner, 2020). For RF we use the quantile regression forest implementation (Meinshausen, 2006) within the R package “ranger” (Wright and Ziegler, 2017), for MLP we use the R package “qrnn” (Cannon, 2024), and for ARX the linear model option in the scikit-learn Python tool.

RNNED is a sequence-to-sequence framework that uses LSTM to encode the history of the input sequence into a context vector and to recursively decode it into predictions (Cho et al., 2014; Hochreiter and Schmidhuber, 1997). Direct multi-horizon forecasting is performed by the decoder generating a sequence of future predictions at once. The encoder is a RNN whose hidden state at the time step when the forecast starts is a summary  $c$  of the whole input sequence, while the decoder is a RNN that generates predictions  $y_t$  based on its hidden state  $h_t$ , the prediction of the previous time step  $y_{t-1}$ , and  $c$ . Note also that  $h_t$  itself is a function of  $y_{t-1}$  and  $c$ , as well as  $h_{t-1}$ .

TFT has an attention-based architecture that integrates information from any time step and captures long-term dependencies in the data through interpretable self-attention layers (Lim et al., 2021). The multi-head attention block adds interpretability by identifying relevant time steps within the encoder period. Local temporal processing is done with LSTMs in the encoder and decoder in a similar manner to the RNNED. The TFT also includes Variable Selection Networks that at each step inform about the importance of the individual predictors and allow the model to neglect irrelevant inputs. Gated Residual Networks (GRN) consisting of two dense layers and an Exponential Linear Unit (ELU) activation function (Clevert et al., 2015) are used within the Variable Selection Networks and elsewhere in the model architecture as gating mechanisms to adapt the model’s depth and complexity according to the task at hand. Note that attention-based approaches are computationally

demanding given that they can explicitly model the interaction between every pair of input-output elements (Challu et al., 2023).

155

Finally, NHITS follows a different approach characterized by multi-rate sampling of the input and hierarchical interpolation of the output to increase computational efficiency, particularly for long-horizon forecasts (Challu et al., 2023). The model is composed of stacks of MLP blocks, with each block capturing a different part of the time series, and with each stack dealing with a different frequency (timescale) of the time series. The stacks range from those with a smooth input and low cardinality output to those with high frequency input and high cardinality output. The forecast over all lead times is assembled by summing the temporally-interpolated outputs of all blocks from all stacks.

160

For all three deep learning models we define the length of the encoder to be 64 days, whereas the forecasting horizon goes up to 32 days. We use 24 forecast creation times every 15 days during the year 2021 as our validation set when training the models. During each epoch of the training, 30 batches of 64 encoder-decoder chains are randomly sampled from the set of time series composed by the data of all 54 stations between 2012 and 2020. At the end of each epoch, the model parameters are updated only if they reduce the average quantile loss over all selected quantiles, lead times, and forecast creation times of the validation set. The quantile loss (QL) is given by Eq. (2), where  $q$  is a quantile,  $y$  is the observed value,  $\hat{y}$  is the prediction, and  $(\cdot)_+ = \max(0, \cdot)$ . Note that the QL averaged over all quantile levels is an approximation of the well-known Continuous Ranked Probability Score (CRPS) (Fakoor et al., 2023; Laio and Tamea, 2007). In the case of RNNED, we use mean absolute error (MAE) instead of QL, because QL is not supported in the source code. Here we decide to stop the training of the models if the parameters are not updated during 60 consecutive epochs, suggesting that they have converged to an optimal value. In addition, to limit computing time we stop the training if a maximum number of 200 epochs is reached. Finally, given that the parameter optimization is not deterministic, we train each deep learning model 10 times with a different random seed.

165

170

175

$$QL = q(y - \hat{y})_+ + (1 - q)(\hat{y} - y)_+ \quad (2)$$

To train the ARX, RF and MLP models we use all data from 2012 to 2021, and their default settings. A least squares fit is done for ARX, whereas QL is used when training the RF and MLP.

180

### 2.3 Model features and hyperparameters

The deep learning models include static catchment characteristics as predictors, given that a single model is fitted for all 54 stations. Here we use all the static features provided in Table S1, i.e. catchment area, mean elevation, glacierized fraction, station coordinates, and long-term average and standard deviation of the target variable (target center and scale). The primary set of known time varying model features used for the analysis includes meteorological variables and time of the year, i.e.

185



AT, P, SD, and DI, as these are commonly available. Additional sets of model features that exclude predictors are also evaluated in section 3.3. Lastly, the models also include observed WT from the encoder period.

One important aspect that influences the predictions of machine learning models is the selection of hyperparameters (e.g. (Feigl et al., 2021; Kraft et al., 2024)). Therefore, we conduct hyperparameter tuning for each of the deep learning models using the Optuna framework (Akiba et al., 2019). Proposed hyperparameter values are iteratively sampled 25 times with a Tree-structured Parzen Estimator (Bergstra et al., 2011) that efficiently explores the hyperparameter space by focusing on the regions with the largest potential to improve the model skill, i.e. to reduce the validation loss. Additionally, hyperband pruning is used to stop early on the iterations with hyperparameters that won't improve skill (Li et al., 2018). Details on the hyperparameters of each model, the explored hyperparameter space, and their tuned values are provided in Table S2.

The ARX, RF and MLP models are trained per station, and hence do not include static features. These models do not encode information from the recent past, so here we include lagged (observed or predicted) water temperature at time  $t-1$  (lagWT) to predict water temperature at time  $t$ . The final set of features includes lagWT, AT, P, SD and DI. We set the RF to 500 trees of unlimited depth, and the MLP to have 1 hidden layer with 2 hidden nodes.

#### 2.4 Forecasting at new and ungauged stations

The capability of a model to generate skillful water temperature forecasts at new locations can be of great added value for stakeholders because long-term measurements are not available everywhere (Ouarda et al., 2022). Given that deep learning models are trained on a set of stations, instead of individual time series, we expect some transferability in space to locations with similar conditions. To analyze the performance of the deep learning models at new stations with water temperature observations and at ungauged locations we consider models with three different setups: (A) our control model trained on all 54 stations, (B) a model trained on a subset of 34 stations with the same features as A, and (C) a model trained on a subset of 34 stations excluding past observations of water temperature from the features (i.e. ungauged). Finally, we compare the predictions of A and B, as well as A and C, across the subset of remaining 20 stations not used when training B and C.

We divide our data into two subsets of 34 and 20 stations with similar distributions of catchment area, mean elevation and glacierized fraction as indicated in Table S1. In addition, we note that for setup B we use an encoder normalizer instead of group normalizer when training the model. This means that the features include the average and standard deviation of water temperature (target center and scale) over the encoder period, as opposed to their long-term average as in A. Meanwhile for setup C, given that we do not include past water temperature as a feature, we also do not include its average and standard deviation.



## 2.5 Model performance evaluation

We use observed stream temperature from the year 2022 (excluded from model training) and 90 forecasts distributed over the year to assess the predictive skill of the models (Table S3). We do so with the Continuous Ranked Probability Score (CRPS), which is designed for ensemble forecasts (e.g. Jolliffe and Stephenson, 2012). The CRPS compares the cumulative distribution function (CDF) of the forecasts against the observations, and it corresponds to the mean absolute error for the case when a single value is predicted. Therefore, the units of the CRPS are those of the observed variable, with values closer to 0 corresponding to a better agreement between predictions and observations.

In our case, for each of the 51 driving meteorological forecasts, the models generate a probabilistic forecast of daily maximum water temperature given by quantiles  $q_2$ ,  $q_{10}$ ,  $q_{25}$ ,  $q_{50}$ ,  $q_{75}$ ,  $q_{90}$  and  $q_{98}$ . First, for each set of quantiles we fit a normal distribution with mean  $\mu = q_{50}$  and standard deviation  $\sigma = (q_{90} - q_{10}) / (sn(q_{90}) - sn(q_{10}))$ ; where  $sn(qX)$  corresponds to the quantile  $X$  of the standard normal distribution (i.e. with a standard deviation of 1). We then sample 100 values from each of the 51 fitted normal distributions and fit a final normal distribution to these data with parameters  $\mu_f$  and  $\sigma_f$ . This final distribution is used when computing the CRPS according to Eq. 3, where  $y$  is the observed value (i.e. daily maximum water temperature),  $\Phi$  is the CDF of the standard normal distribution, and  $\phi$  is probability density function of the standard normal distribution.

$$CRPS = \sigma_f \left( \frac{y - \mu_f}{\sigma_f} \left( 2\Phi \left( \frac{y - \mu_f}{\sigma_f} \right) - 1 \right) + 2\phi \left( \frac{y - \mu_f}{\sigma_f} \right) - \frac{1}{\sqrt{\pi}} \right) \quad (3)$$

## 3 Results and discussion

### 3.1 Model performance comparison

We first compare the predictive skill of the models omitting the uncertainty stemming from the meteorological forecasts of AT, P, and SD, i.e. when using their observed values instead of their forecasts over the 32 days of the prediction horizon (Fig. 2). The TFT performs best with an average CRPS of 0.39 °C over all random seeds, lead times, stations, and forecast start dates. The other deep learning models RNNED (0.57 °C) and NHITS (0.60 °C) are next in line, closely followed by the RF (0.64 °C) and MLP (0.66 °C). For the simplest linear ARX model the CRPS degrades to 0.97 °C, which is 0.58 °C worse than that of the TFT. The deep learning models show little spread in their average CRPS across the 10 random seeds: 0.014 °C for the TFT, 0.040 °C for the RNNED, and 0.022 °C for the NHITS. This suggests the models converged to optimal parameters during training. Regarding the run time needed on our server to train each model for 200 epochs, the longest is 44 minutes for the TFT with 286.1k parameters, followed by 21 minutes for the RNNED with 60.9k parameters, and 17 minutes

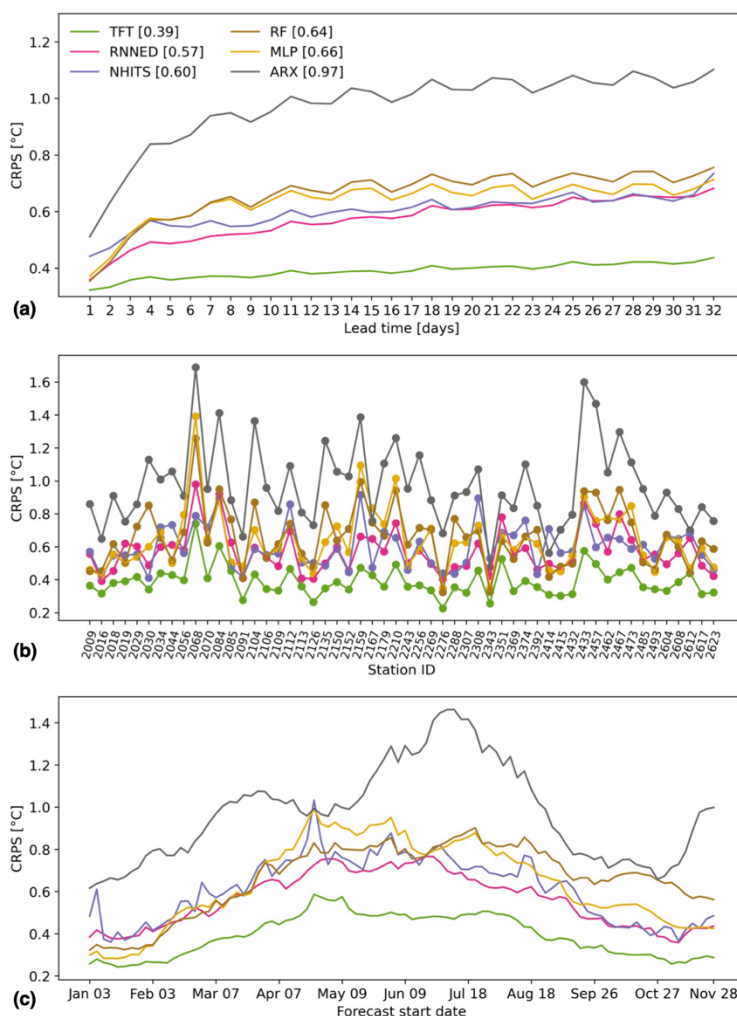




for the NHITS with 103.8k parameters. For the simpler models less than a minute is needed to train them at each station, and this can easily be done in parallel.

For all models the predictive skill decreases with lead time, as the influence of observed daily maximum water temperature on the predictions also reduces (Fig. 2a). The decrease in skill is particularly fast during the first 4 days for ARX, MLP and RF, suggesting that these models have a higher reliance on past water temperature for predicting future water temperature. Across stations, there is substantial variability in the CRPS for all models (Fig. 2b). As an example for the TFT, it ranges from 0.23 °C for station 2276 (Grosstalbach – Isenthal) to 0.74 °C for station 2068 (Ticino – Riazzino). No clear relationships emerge when evaluating predictive skill as a function of catchment characteristics such as area, elevation and glacierized fraction (Fig. S1). Lastly, we note that the predictive skill of the models also varies seasonally (Fig. 2c). The CRPS is lower in the winter when water temperature is colder and has lower day-to-day variability, whereas it is higher in the summer when the conditions are opposite.

It is likely that stream water temperature at several of the Swiss stations analyzed in this study is influenced by reservoir and lake management (Michel et al., 2020), and potentially also by water withdrawal and discharge from industry for example. Larger deviations between observed and forecasted values are expected when management decisions influencing water temperature take place, given that their timing can be largely arbitrary, and thus not captured by our models. This seems to be the case for stations 2068 (Ticino – Riazzino), 2084 (Muota – Ingenbohl), and 2351 (Vispa – Visp) with the highest CRPS as seen in Fig. 2b. These stations are highly influenced by hydropeaking from the release of large volumes of cold water from reservoirs at high elevation (Michel et al., 2020). It is noteworthy that the high CRPS values for forecast-start-dates between mid-April to mid-May (Fig. 2c) are mainly driven by high CRPS values at these affected stations (Fig. S2). Furthermore, during this time of the year 2022 the models underestimate the observed water temperatures (Fig. S3), which is a reasonable consequence if less cold water was released during the drought year 2022 compared to past years used to train the models.



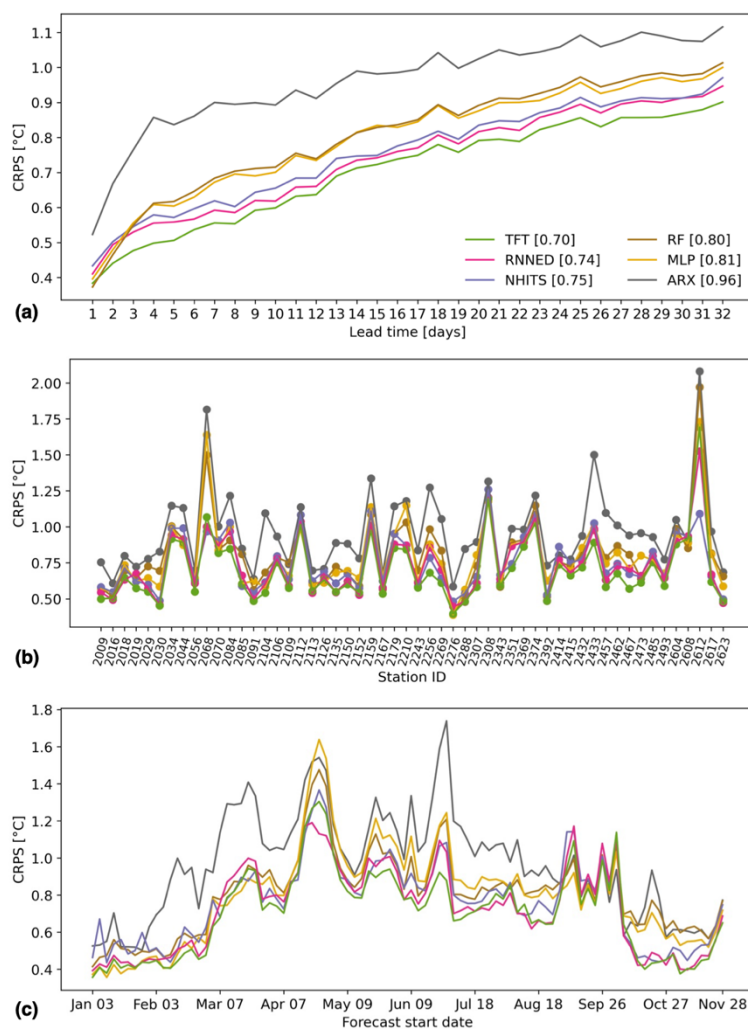
270

**Figure 2: Model comparison of predictive skill when omitting the uncertainty of meteorological forecasts.** The cumulative rank probability score (CRPS) of each model is shown as a function of (a) lead time averaged over all stations and forecasts, (b) station averaged over all lead times and forecasts, and (c) forecast start date averaged over all lead times and stations. The legend indicates the different models and their average CRPS over all 32 lead times, 54 stations, and 90 forecasts distributed over the year 2022.

275 Figure 3 compares the operational predictive skill of the models when using AT, P, and SD forecasts over the 32 days of the prediction horizon. The TFT remains the best performing model with an average CRPS of 0.70 °C over all random seeds, lead times, stations, and forecast start dates, followed by RNNED with 0.74 °C, NHITS with 0.75 °C, RF with 0.80 °C, MLP with 0.81 °C, and ARX with 0.96 °C. When comparing these results to those from Fig. 2, we note that the uncertainty of the meteorological forecasts contributes 0.31 °C to the total disagreement between observations and TFT predictions, and less  
 280 for the other models. Consequently, the uncertainty of the meteorological forecasts decreases the gain in predictive skill to be achieved when using the TFT compared to the other models. This is particularly the case for lead times beyond 5 days when there is often a strong decrease in meteorological predictability (Bauer et al., 2015).



285 There is an evident decrease in predictive skill of water temperature as lead time increases (Fig. 3a), which is directly related to the ensemble meteorological forecasts being less accurate and having a larger spread for predictions further into the future. For all models, the CRPS at a lead time of 32 days is more than double its value at a lead time of 1 day. In the case of the TFT it increases from 0.38 °C at lead time 1 to 0.90 °C at lead time 32. In addition, we find that the uncertainty of the meteorological forecasts increases the CRPS variability across stations and forecast start dates, and can lead to other models outperforming the TFT in some cases (Figs. 3b and 3c).



290

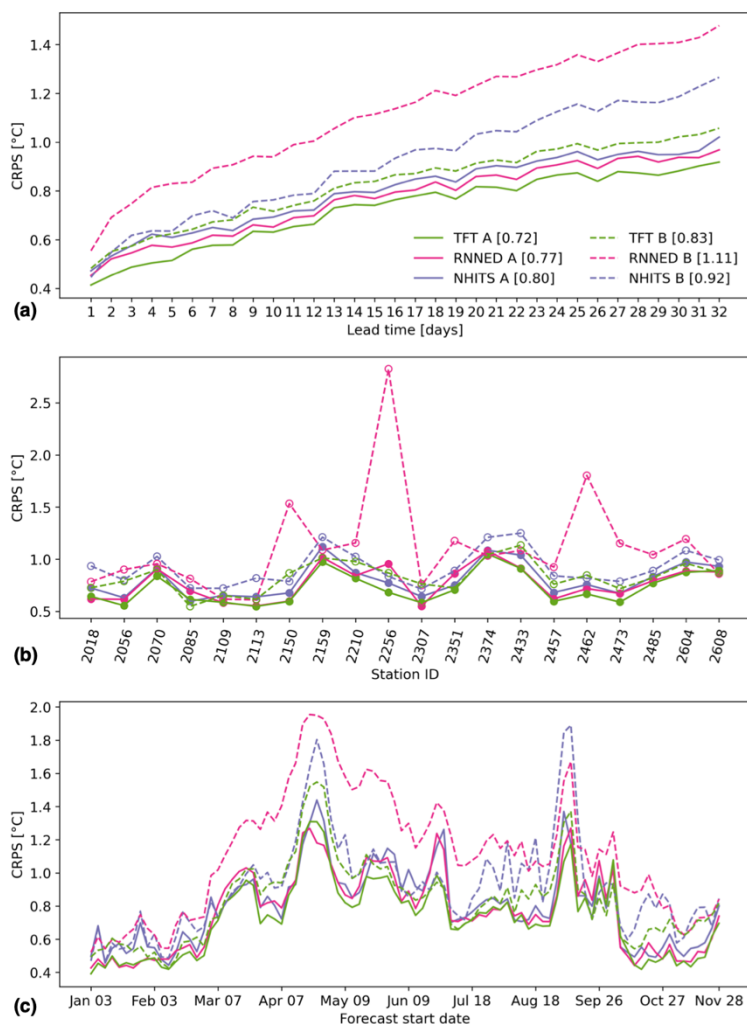
**Figure 3: Model comparison of predictive skill when including the uncertainty of meteorological forecasts.** The cumulative rank probability score (CRPS) of each model is shown as a function of (a) lead time averaged over all stations and forecasts, (b) station averaged over all lead times and forecasts, and (c) forecast start date averaged over all lead times and stations. The legend indicates the different models and their average CRPS over all 32 lead times, 54 stations, and 90 forecasts distributed over the year 2022.



295 High average CRPS values greater than 1 °C – even for the TFT – occur at several stations: 2612 (Riale di Pincascia –  
Lavertezzo), 2308 (Goldach - Goldach, Bleiche, nur Hauptstation), 2068 (Ticino – Riazzino), 2374 (Necker – Mogelsberg,  
Aachsäge), and 2112 (Sitter – Appenzell), representing a large increase compared to their values in Figure 2 (except for  
station 2068 influenced by reservoir management). Therefore, these high errors in predicted water temperature arise from  
errors in the meteorological forecasts. Furthermore, the catchment area of the above-mentioned stations is less than 90 km<sup>2</sup>  
300 (except station 2068), and the catchment of station 2612 is particularly steep. These conditions are likely to make water  
temperature more sensitive to changes in AT, P, and SD – i.e. the change in water temperature per unit change in the  
meteorological predictors is greater (e.g. Wade et al., 2023). Figure S4 indeed shows a tendency for higher CRPS at stations  
with smaller catchment area. Finally, the high CRPS values during April and September in Figure 3c result from the  
contribution of most stations (with a strong influence from station 2612) (Fig. S5). This decrease in predictive skill was  
305 caused by specific weather events that deviated strongly from the meteorological forecasts, particularly for lead times  
beyond two weeks (Fig. S6).

### 3.2 Predictive skill at new and ungauged stations

Figure 4 compares the CRPS across 20 stations from predictions of deep learning models trained either including (setup A)  
or excluding (setup B) data from this subset of stations. When forecasting water temperature at new stations on which the  
310 models are not trained, results show that the TFT performs best with an average CRPS of 0.83 °C across all 32 lead times, 20  
stations, and 90 forecast start dates, followed by the NHITS with 0.92 °C, and the RNNED with 1.11 °C. The reduction in  
prediction skill when extrapolating the models to new stations is 0.11 °C for the TFT, 0.12 °C for the NHITS, and 0.34 °C for  
the RNNED. The larger drop in skill of the RNNED occurs at more than half of the 20 stations and throughout most forecast  
dates, with particularly large values at the highest elevation stations: 2256 (Rosegbach – Pontresina) and 2462 (Inn – S-  
315 chanf). On the other hand, we note the good extrapolation capability of the TFT to new stations during the summer, with its  
CRPS following closely that of the TFT trained on all 54 stations.



**Figure 4: Model comparison of predictive skill at new stations.** Continuous lines correspond to setup A when models are trained on data from all 54 stations, whereas dashed lines correspond to setup B when models are trained on data excluding the subset of 20 stations. The cumulative rank probability score (CRPS) of each model is shown as a function of (a) lead time averaged over subset of 20 stations and all forecasts, (b) station averaged over all lead times and forecasts, and (c) forecast start date averaged over all lead times and subset of 20 stations. The legend indicates the different models and their average CRPS over all 32 lead times, 20 stations, and 90 forecasts distributed over the year 2022.

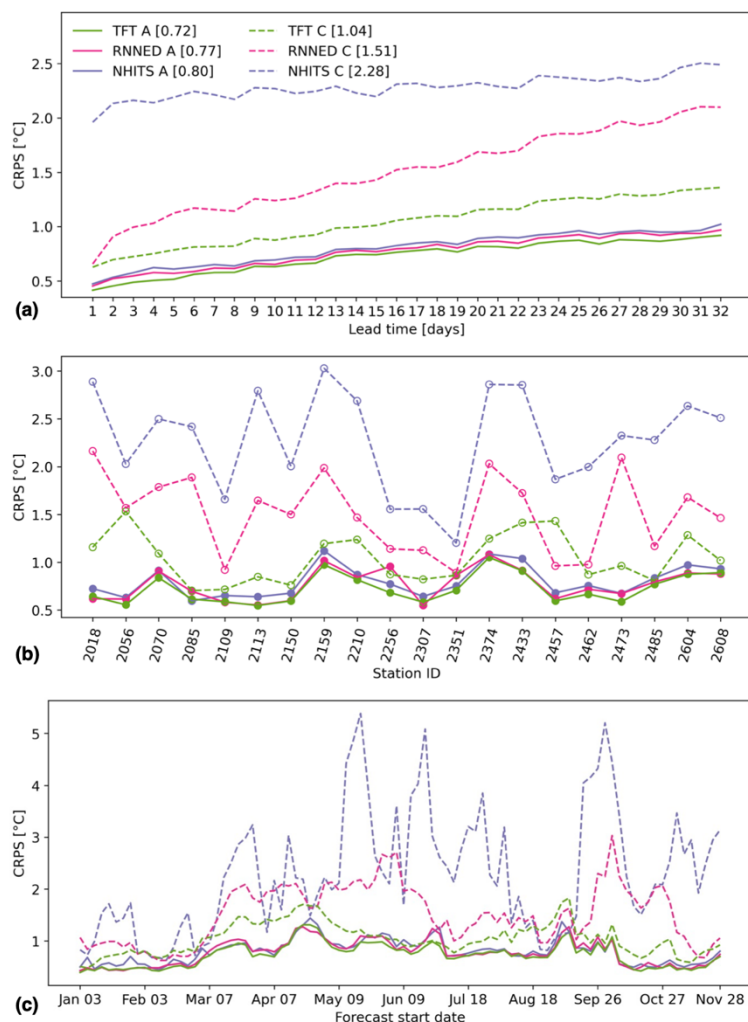
320

There is a clear decrease in prediction skill across the 20 stations when forecasting with models that exclude information on past water temperature, and that are trained omitting the data from these stations (setup C) – as to represent ungauged stations (Fig. 5). Nonetheless, the TFT is still able to achieve an average CRPS of 1.04 °C across all 32 lead times, 20 stations, and 90 forecast start dates, which corresponds to a reduction in prediction skill of 0.32 °C compared to the model that includes past observations of water temperature and is trained using data from all 54 stations. Up to two weeks of lead time, the TFT average CRPS at ungauged stations is below 1 °C. Furthermore, the CRPS of the TFT is lower than that of the RNNED and NHITS across almost all 20 stations and 90 forecast start dates. On the other hand, it is evident that the NHITS

330



model is not well-suited to generate predictions at ungauged stations as it strongly relies on past observations of the target variable to forecast future values.



335 **Figure 5: Model comparison of predictive skill at ungauged stations.** Continuous lines correspond to setup A when models include past  
 observations of water temperature as a feature and are trained on data from all 54 stations, whereas dashed lines correspond to setup C  
 when models exclude past observations of water temperature as a feature and are trained on data excluding the subset of 20 stations. The  
 cumulative rank probability score (CRPS) of each model is shown as a function of **(a)** lead time averaged over subset of 20 stations and all  
 340 forecasts, **(b)** station averaged over all lead times and forecasts, and **(c)** forecast start date averaged over all lead times and subset of 20  
 stations. The legend indicates the different models and their average CRPS over all 32 lead times, 20 stations, and 90 forecasts distributed  
 over the year 2022.

### 3.3 Predictive importance of model inputs

Here we focus on the TFT given that it outperforms the other models, and because of its built-in interpretability (Lim et al., 2021). For every forecast, the TFT directly outputs fractional importance weights (*importance*) that sum up to 1 for static features, for encoder features, and for decoder features separately. On average across the 10 random seeds and 54 stations,



345 results show similar *importance* values for all static features (Fig. S7). Target center (i.e. the long-term average of daily maximum water temperature) with 0.16 has the highest *importance*, whereas catchment area with 0.09 has the lowest *importance*. For individual stations, features with higher *importance* are typically those that differentiate them from other stations. For example, the importance of catchment glacierized fraction increases for stations with higher glacierized fraction.

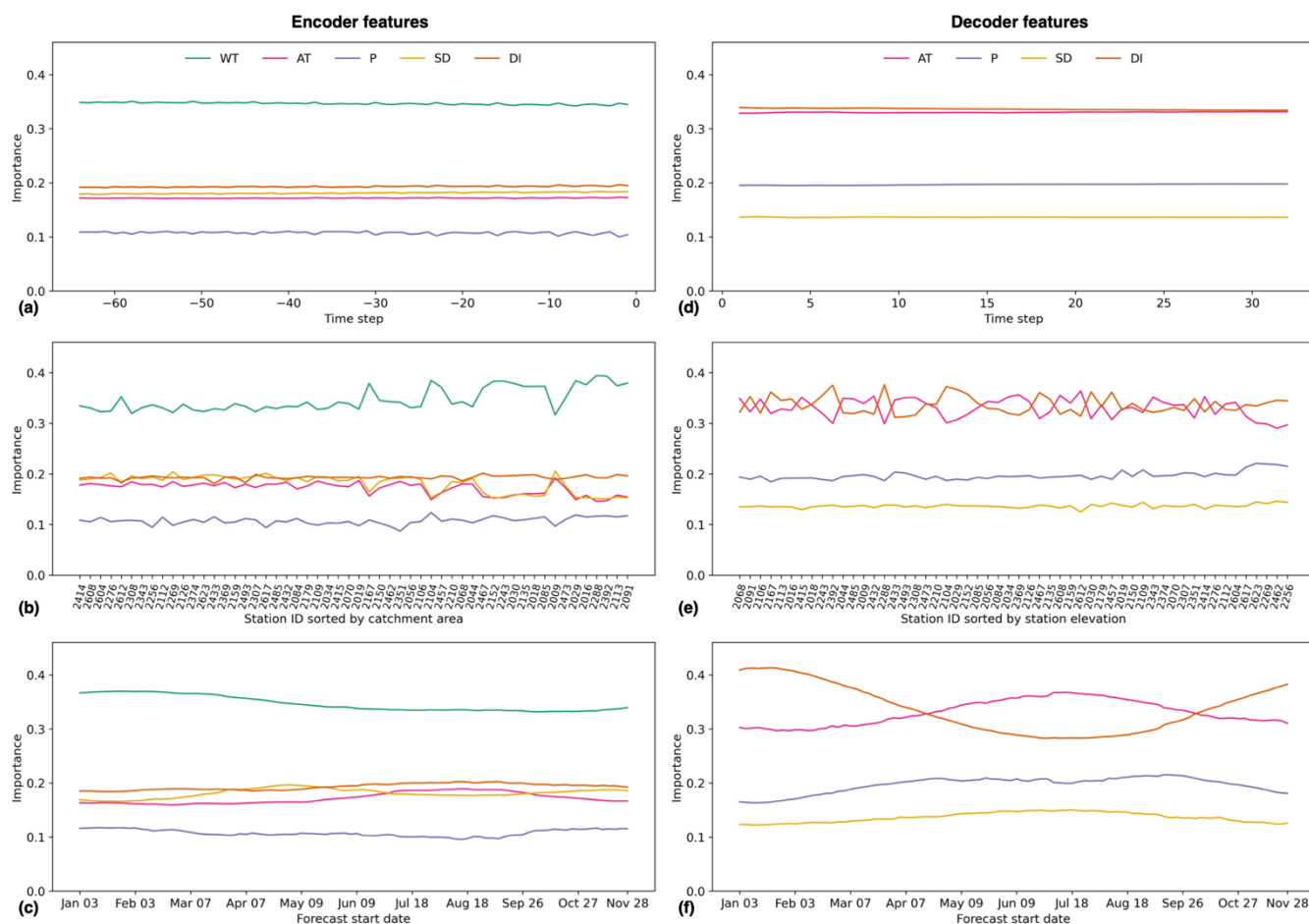
350

Figure 6 shows WT has the highest *importance* among the encoder features with an average value of 0.35 over all random seeds, encoder time steps, stations, and forecasts. AT, SD, and DI have similar *importance* values of 0.17, 0.18, and 0.19, respectively, whereas P with 0.11 has the lowest. There is very low *importance* variability of the encoder features across time steps, stations and forecast start date. Nevertheless, we note a slightly higher *importance* of WT at larger catchments, and a small increase in the *importance* of AT for forecasts in July and August. For the decoder features, AT and DI have the highest average *importance* with a value of 0.33, followed by P with 0.20, and SD with 0.14. These weights are almost constant for all decoder time steps. Across stations, we find that approximately in half of them AT is slightly more important than DI, whereas the opposite is true for the remaining half. Also, there is a small but noteworthy increase in P *importance* at high elevation stations at the expense of AT. Lastly, results suggest that DI is generally more important for forecasts during the cold months, whereas the *importance* of AT, P, and SD increases during the warm months.

360

When interpreting the *importance* weights, it is useful to acknowledge that the model features are clearly not independent from one another. The meteorological features correlate with DI due to their seasonality. Higher SD is expected to coincide with higher AT, particularly during the warmer months. In addition, cloudiness influences the number of sunny hours and is a prerequisite for precipitation, thus relating SD and P. Consequently, the feature *importance* values can vary substantially every time the TFT model is trained with a different random seed (Fig. S8), even though the predictive skill hardly changes. In an operational context, the *importance* weights are nonetheless relevant to shed light on which meteorological conditions influence the model more every time a new forecast of daily maximum water temperature is generated.

365



370

**Figure 6: TFT feature importance.** The *importance* of each feature is shown as a function of (a,d) time step averaged over all stations and forecasts, (b,e) station averaged over all time steps and forecasts, and (c,f) forecast start date averaged over all time steps and stations. Encoder feature *importance* is shown in (a,b,c) and decoder feature *importance* in (d,e,f). Note that in (b) stations are sorted by catchment area in ascending order, and in (e) stations are sorted by station elevation in ascending order. In all cases the *importance* is averaged across

375

10 models trained with different random seeds.

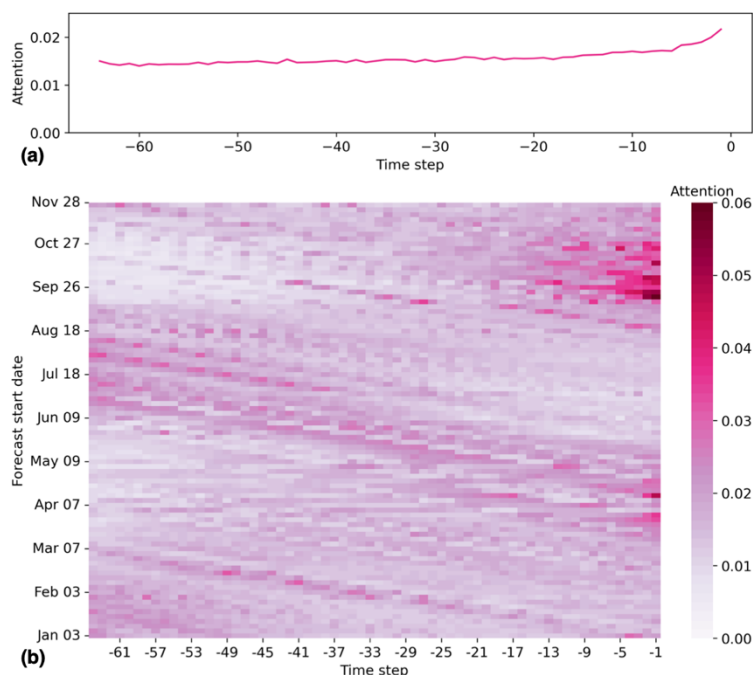
The TFT also provides fractional attention weights (*attention*) that sum up to 1 and indicate the relevance of information from different encoder time steps for the forecasts. On average, *attention* is highest for the most recent 5 days leading up to the forecast date, and then rather similar from time step -6 to -64 (Fig. 7a). Notably, forecast start dates in the Spring and Autumn tend to have higher *attention* to the most recent days (Fig. 7b). Furthermore, it is evident how the high *attention* to recent time steps for forecasts starting in March and April, propagates to time steps further back in time over the next forecast start dates. This suggests that the values of the encoder features (WT, AT, P, SD, and DI) in Spring remain relevant for forecast start dates up to 64 days later at the end of June. Given that *attention* weights are influenced by the *importance* of the model's encoder features, there is also significant *attention* variability for models trained with different random seeds

380





(Fig. S9). Typically, the relative *attention* to time steps further back in time increases when WT and DI have higher *importance*, whereas *attention* to most recent time steps tends to increase when the model relies more on AT and SD.

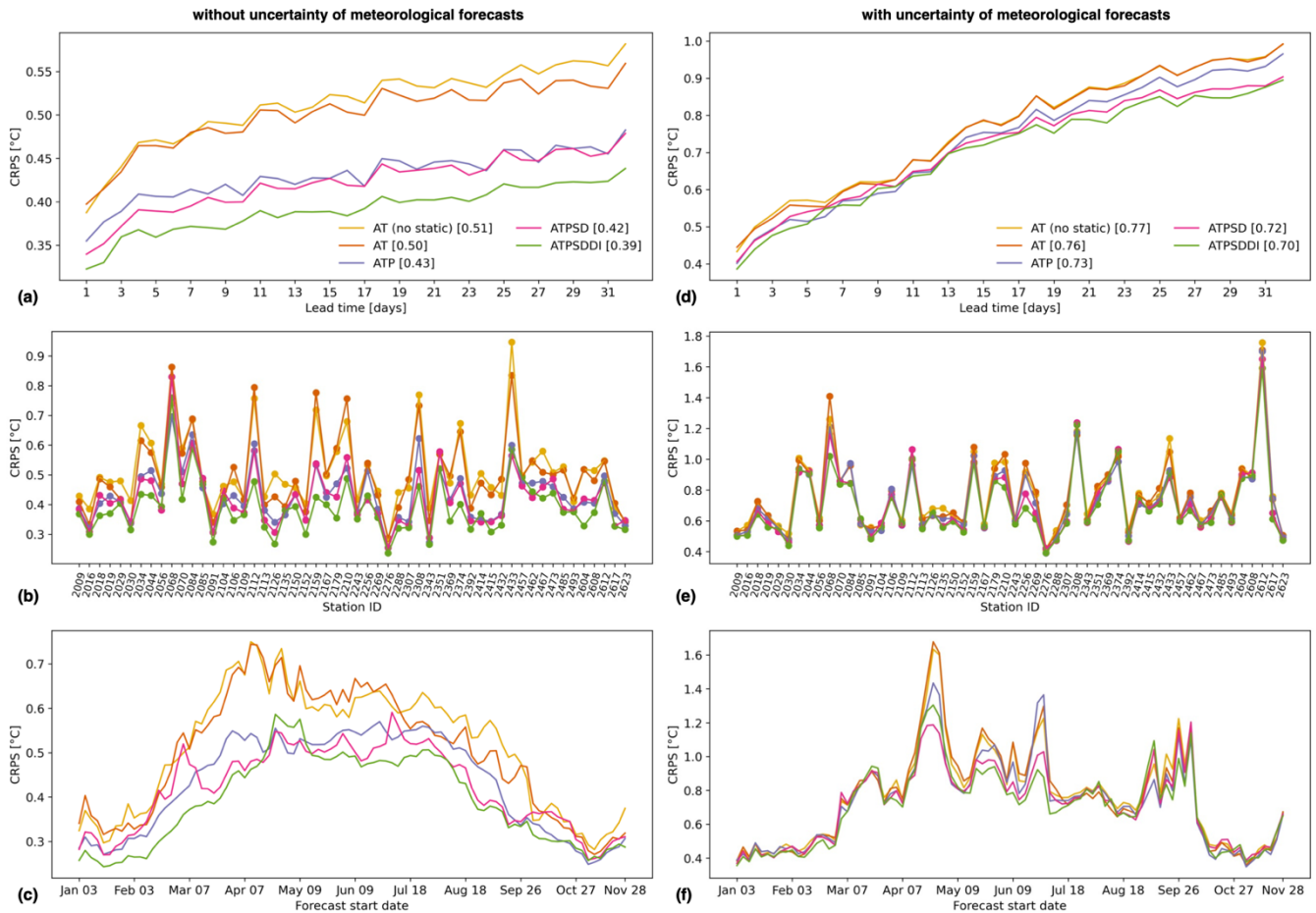


**Figure 7: TFT attention weights to encoder time steps. (a)** *Attention* averaged across random seeds, stations, and forecast start dates as a function of encoder time step. **(b)** *Attention* averaged across random seeds and stations as a function of encoder time step and forecast start date.

In addition to the TFT *importance* weights, here we compare the predictive skill of TFT models with different sets of predictor features (Fig. 8). When omitting the uncertainty of meteorological forecasts, results show a good average CRPS of 0.51 °C for the simplest model with the following predictors: long-term average and standard deviation of WT (target center and scale) from each station as static features, encoder period WT, and AT. With each new predictor included in the model, the CRPS improves incrementally across almost all lead times, stations and forecasts, reaching an average of 0.39 °C for the most complex model with catchment static features, P, SD, and DI as additional predictors. The largest gain in predictive skill is obtained when adding P as a predictor, with the improvement taking place mostly at stations of small and low elevation catchments, as well as being particularly high in Spring. Given that smaller catchments tend to have less streamflow, precipitation events could more easily influence upstream water mixing and consequently station water temperature. Also, in Spring we expect larger water temperature differences between contributing sources such as rainfall runoff, snowmelt, and lake discharge. In addition to P, the inclusion of DI also clearly improves predictive skill by capturing seasonal characteristics of water and heat fluxes in the catchments. Overall, our findings are consistent with previous studies noting the relevance of precipitation or runoff, as well as global radiation and time of the year for predicting stream water temperature (e.g. Feigl et al., 2021; Zhu and Piotrowski, 2020).



405 The biases and spread of the ensemble meteorological forecasts limit the gain in predictive skill as more predictors are included in the TFT models. The average CRPS improves from 0.77 °C for the simplest model to 0.70 °C for the model with static features, WT (encoder period), AT, P, SD, and DI. Nevertheless, adding SD forecasts is particularly beneficial to improve model skill for lead times longer than 3 weeks, and at high elevation stations such as 2256 (Rosegbach – Pontresina), 2269 (Lonza – Blatten), 2612 (Riale di Pincascia – Lavertezzo), and 2617 (Rom – Müstair). Lastly, we note that including SD and DI is especially beneficial for forecast start dates from mid-April to end of June.



410

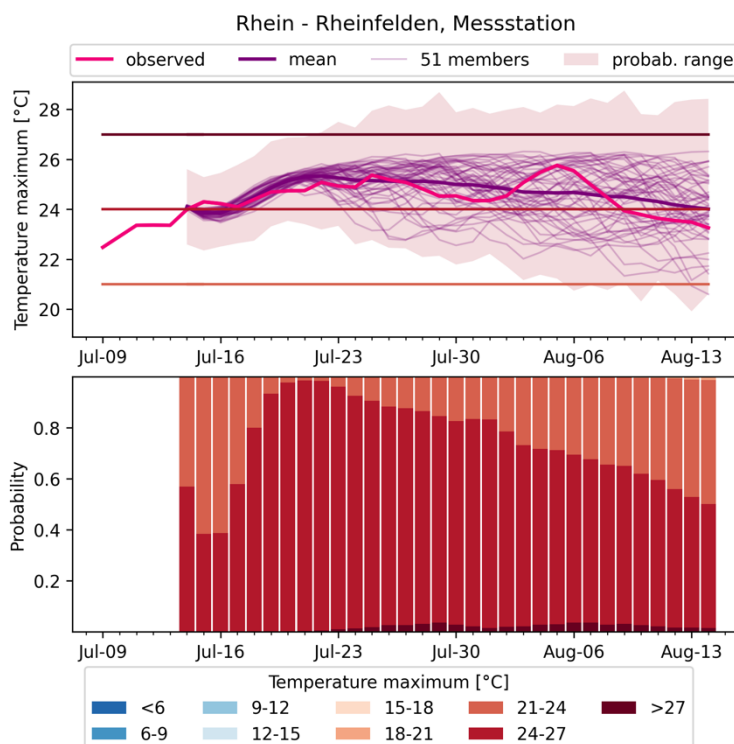
**Figure 8: Predictive skill comparison of TFT models with different features.** The cumulative rank probability score (CRPS) of each model is shown as a function of (a,d) lead time averaged over all stations and forecasts, (b,e) station averaged over all lead times and forecasts, and (c,f) forecast start date averaged over all lead times and stations. The CRPS is shown when computed omitting the uncertainty of meteorological forecasts (a,b,c), and when computed including the uncertainty of meteorological forecasts (d,e,f). The legend indicates the different models and their average CRPS over all 32 lead times, 54 stations, and 90 forecasts distributed over the year 2022. “AT (no static)” includes long-term average and standard deviation of WT (target center and scale) from each station as static features, encoder period WT, and AT. “AT” has the same features plus catchment static features (i.e. station coordinates, area, mean elevation, and glacierized fraction). “ATP” adds P as predictor, “ATPSD” adds SD, and “ATPSDDI” adds DI.

415

### 3.4 Operational forecasts

420 Extended range probabilistic forecasts of daily maximum water temperature at the 54 stations in Switzerland are generated operationally twice per week and made available at <https://www.drought.ch/de/impakt-vorhersagen-malefix/wassertemperatur-prognosen/>. The best performing TFT model with static catchment features, AT, P, SD, DI, and past WT as predictors is used. Figure 9 shows an example forecast for station 2091 (Rhein – Rheinfelden, Messstation) generated on 14 July 2022. Estimates based on each of the 51 ECMWF members provide insight on the expected uncertainty driven by the meteorological forecasts. The ensuing observations follow closely the best estimate forecast during the first 7 days of lead time and remain within range up to the maximum lead time of 32 days.

It is the aim that stakeholders benefit from our timely forecasts for their decision-making. As a concrete example, an early warning system for fish thermal stress was developed using the stream water temperature forecasts as input  
430 (<https://www.drought.ch/de/impakt-vorhersagen-malefix/risiko-von-thermischem-stress-fuer-fische/>). High stream water temperatures pose a grave threat to fish populations (Barbarossa et al., 2021), as experienced during the summer of 2018 in Switzerland when tons of fish died in the Rhein. Therefore, timely knowledge on the exceedance potential of dangerous water temperature thresholds as given in Figure 9 is important. The July 14 forecast indicated occurrence probabilities generally greater than 60% for daily maximum stream water temperature to rise above 24 °C at station 2091 over the coming  
435 weeks, which was then the case from July 14 to August 8.





440 **Figure 9: Operational daily maximum water temperature forecast on 14 July 2022 at station 2091 (Rhein – Rheinfelden, Messstation).** The forecast is generated with the best performing TFT model with static catchment features, AT, P, SD, DI, and past WT as predictors. The temporal evolution of observed water temperature is shown at the top panel together with the forecast best estimate, the 51 estimates based on each of the ECMWF ensemble members of the meteorological forecast, and the probability range. The bottom panel shows the daily forecast probability for different categories of daily maximum water temperature.

#### 4 Conclusions

In this study we evaluate state-of-the-art deep learning models for stream water temperature predictions over the next 32 days, given the high value of skillful probabilistic extended range forecasts for managerial decisions. Deep learning models go beyond the iterative predictions of their standard counterparts, by efficiently generating instead direct multi-horizon forecasts across multiple stations at once. The TFT model performs best with an average CRPS of 0.70 °C, degrading from 0.38 °C at 1 day lead time to 0.90 °C at 32 days lead time. We find that 0.31 °C of the average disagreement between observations and predictions stems from the uncertainty in the meteorological forecasts of AT, P, and SD. This is a novel insight on the current limits of extended range water temperature predictability.

450 The 54 stream water temperature stations from the Swiss Federal Office for the Environment monitoring network comprise catchments varying in size, elevation, steepness, and different degrees of human interventions. These data are exploited by the deep learning algorithms to generalize the relationships between water temperature and its predictors. Our results demonstrate the potential of the TFT model to predict water temperature at stations on which it was not trained, and at ungauged locations. The error at new stations increases 0.11 °C reaching an average CRPS of 0.83 °C, whereas it increases to 1.04 °C when local water temperature is unavailable to the model. This is an important step forward in the quest to expand the availability of stream water temperature estimates across the world. Furthermore, the TFT model may also be used to generate predictions under future climate scenarios assuming no major changes on how water temperature responds to changes in the meteorological drivers.

460 Our detailed analysis of the importance of different model inputs highlights the roles of WT in the encoder period, AT and DI in the decoder period, and of the station specific long-term average of daily maximum water temperature among the static features. The TFT model with only WT and AT as time-varying inputs performs well with an average CRPS of 0.76 °C, which improves to 0.70 °C when including P, SD, and DI. Overall, the TFT insights on feature importance and attention to encoder period time steps for each forecast provide valuable interpretability that was often missing in machine learning models.

470 The publicly available operational system for extended range forecasts of daily maximum water temperature completes our contribution by regularly providing information to parties interested on the consequences of extreme conditions. The methodology, insights, and product of this study help address the growing challenges surrounding stream water temperatures



– and consequently water quality – in our warming world. Finally, we underscore the necessity for more and better information on this key environmental variable.

### **Code and data availability**

The meteorological data used in this study can be requested from the Swiss Federal Office for Meteorology and  
475 Climatology, whereas the water temperature data can be requested from the Swiss Federal Office for the Environment.  
Scripts used in this study will be available upon final publication.

### **Author contributions**

RSP, MZ, and KB conceived the idea and designed the study. RSP performed the analysis and wrote the paper with  
suggestions from MZ and KB. LB led the implementation of the operational forecasts and provided technical support. KB  
480 contributed to the analysis. All authors read and reviewed the paper.

### **Competing interests**

The authors declare that they have no conflict of interest.

### **Acknowledgements**

We acknowledge support from the MaLeFix project within the EXTREMES programme of the Swiss Federal Institute for  
485 Forest, Snow and Landscape Research WSL. We acknowledge the Swiss Federal Office for Meteorology and Climatology  
and the Swiss Federal Office for the Environment for providing the meteorological and water temperature data, respectively.

### **References**

Akiba, T., Sano, S., Yanase, T., Ohta, T., and Koyama, M.: Optuna: A Next-generation Hyperparameter Optimization  
Framework, in: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining,  
490 KDD '19, pp. 2623–2631, Association for Computing Machinery, New York, NY, USA, ISBN 978-1-4503-6201-6,  
<https://doi.org/10.1145/3292500.3330701>, 2019.

Alfonso, S., Gesto, M., and Sadoul, B.: Temperature increase and its effects on fish stress physiology in the context of global  
warming, *J Fish Biol*, 98, 1496–1508, <https://doi.org/10.1111/JFB.14599>, 2021.

495



Arora, R., Tockner, K., and Venohr, M.: Changing river temperatures in northern Germany: trends and drivers of change, *Hydrol Process*, 30, 3084–3096, <https://doi.org/10.1002/HYP.10849>, 2016.

500 Barbarossa, V., Bosmans, J., Wanders, N., King, H., Bierkens, M. F. P., Huijbregts, M. A. J., and Schipper, A. M.: Threats of global warming to the world's freshwater fishes, *Nature Communications* 2021 12:1, 12, 1–10, <https://doi.org/10.1038/s41467-021-21655-w>, 2021.

505 Bauer, P., Thorpe, A., and Brunet, G.: The quiet revolution of numerical weather prediction, *Nature* 2015 525:7567, 525, 47–55, <https://doi.org/10.1038/nature14956>, 2015.

Beitner, J.: PyTorch Forecasting Documentation, <https://pytorch-forecasting.readthedocs.io/en/stable/#>, 2020.

510 Benyahya, L., Caissie, D., St-Hilaire, A., Ouarda, T. B. M. J., and Bobée, B.: A Review of Statistical Water Temperature Models, *Canadian Water Resources Journal*, 32, 179–192, <https://doi.org/10.4296/CWRJ3203179>, 2007.

Bergstra, J., Bardenet, R., Bengio, Y., and Kégl, B.: Algorithms for Hyper-Parameter Optimization, *Adv Neural Inf Process Syst*, 24, 2011.

515 Bogner, K., Chang, A. Y. Y., Bernhard, L., Zappa, M., Monhart, S., and Spirig, C.: Tercile Forecasts for Extending the Horizon of Skillful Hydrological Predictions, *J Hydrometeorol*, 23, 521–539, <https://doi.org/10.1175/JHM-D-21-0020.1>, 2022.

Booker, D. J., Whitehead, A. L., Doug Booker, C. J., and Modelling, F.: River water temperatures are higher during lower flows after accounting for meteorological variability, *River Res Appl*, 38, 3–22, <https://doi.org/10.1002/RRA.3870>, 2022.

520 Cannon, A.: qrn: Quantile Regression Neural Network. R package, version 2.1.1, <https://CRAN.R-project.org/package=qrn>, 2024.

525 Caretta, M.A., A. Mukherji, M. Arfanuzzaman, R.A. Betts, A. Gelfan, Y. Hirabayashi, T.K. Lissner, J. Liu, E. Lopez Gunn, R. Morgan, S. Mwangi, and S. Supratid.: Water. In: *Climate Change 2022: Impacts, Adaptation and Vulnerability*. Contribution of Working Group II to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [H.-O. Pörtner, D.C. Roberts, M. Tignor, E.S. Poloczanska, K. Mintenbeck, A. Alegría, M. Craig, S. Langsdorf, S. Löschke, V. Möller, A. Okem, B. Rama (eds.)]. Cambridge University Press, Cambridge, UK and New York, NY, USA, pp. 551–712, doi:10.1017/9781009325844.006, 2022.



530

Challu, C., Olivares, K. G., Oreshkin, B. N., Ramirez, F. G., Mergenthaler-Canseco, M., and Dubrawski, A.: NHITS: Neural Hierarchical Interpolation for Time Series Forecasting, *Proceedings of the AAAI Conference on Artificial Intelligence*, 37, 6989–6997, <https://doi.org/10.1609/AAAI.V37I6.25854>, 2023.

535

Chang, A. Y. Y., Bogner, K., Grams, C. M., Monhart, S., Domeisen, D. I. V., and Zappa, M.: Exploring the Use of European Weather Regimes for Improving User-Relevant Hydrological Forecasts at the Subseasonal Scale in Switzerland, *J Hydrometeorol*, 24, 1597–1617, <https://doi.org/10.1175/JHM-D-21-0245.1>, 2023.

540

Chapra, S. C., Camacho, L. A., and McBride, G. B.: Impact of Global Warming on Dissolved Oxygen and BOD Assimilative Capacity of the World's Rivers: Modeling Analysis, *Water* 2021, Vol. 13, Page 2408, 13, 2408, <https://doi.org/10.3390/W13172408>, 2021.

545

Cho, K., Van Merriënboer, B., Gulcehre, C., Bahdanau, D., Bougares, F., Schwenk, H., and Bengio, Y.: Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation, *EMNLP 2014 - 2014 Conference on Empirical Methods in Natural Language Processing, Proceedings of the Conference*, 1724–1734, <https://doi.org/10.3115/v1/d14-1179>, 2014.

550

Clevert, D. A., Unterthiner, T., and Hochreiter, S.: Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs), *4th International Conference on Learning Representations, ICLR 2016 - Conference Track Proceedings*, 2015.

555

Comer-Warner, S. A., Gooddy, D. C., Ullah, S., Glover, L., Percival, A., Kettridge, N., and Krause, S.: Seasonal variability of sediment controls of carbon cycling in an agricultural stream, *Science of The Total Environment*, 688, 732–741, <https://doi.org/10.1016/J.SCITOTENV.2019.06.317>, 2019.

555

Dugdale, S. J., Hannah, D. M., and Malcolm, I. A.: River temperature modelling: A review of process-based approaches and future directions, *Earth Sci Rev*, 175, 97–113, <https://doi.org/10.1016/J.EARSCIREV.2017.10.009>, 2017.

560

Elliott, J. M. and Elliott, J. A.: Temperature requirements of Atlantic salmon *Salmo salar*, brown trout *Salmo trutta* and Arctic charr *Salvelinus alpinus*: predicting the effects of climate change, *J Fish Biol*, 77, 1793–1817, <https://doi.org/10.1111/J.1095-8649.2010.02762.X>, 2010.

Fakoor, R., Kim, T., Mueller, J., Cleanlab, J. A., Smola, A. J., and Tibshirani, R. J.: Flexible model aggregation for quantile regression, *The Journal of Machine Learning Research*, 24, 1–45, <https://doi.org/10.5555/3648699.3648861>, 2023.



565 Fan, C., Zhang, Y., Pan, Y., Li, X., Zhang, C., Yuan, R., Wu, D., Wang, W., Pei, J., and Huang, H.: Multi-horizon time series forecasting with temporal attention learning, *Proceedings of the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 2527–2535, <https://doi.org/10.1145/3292500.3330662>, 2019.

570 Feigl, M., Lebedzinski, K., Herrnegger, M., and Schulz, K.: Machine-learning methods for stream water temperature prediction, *Hydrol Earth Syst Sci*, 25, 2951–2977, <https://doi.org/10.5194/HESS-25-2951-2021>, 2021.

Ficklin, D. L., Hannah, D. M., Wanders, N., Dugdale, S. J., England, J., Klaus, J., Kelleher, C., Khamis, K., and Charlton, M. B.: Rethinking river water temperature in a changing, human-dominated world, *Nature Water* 2023 1:2, 1, 125–128, <https://doi.org/10.1038/s44221-023-00027-2>, 2023.

575

Hannah, D. M. and Garner, G.: River water temperature in the United Kingdom: Changes over the 20th century and possible changes over the 21st century, *Prog Phys Geogr*, 39, 68–92, <https://doi.org/10.1177/0309133314550669>, 2015.

580 Hannah, D. M., Webb, B. W., and Nobilis, F.: River and stream temperature: dynamics, processes, models and implications - preface, *Hydrol Process*, 22, 899–901, 2008.

Hannah, D. M., Demuth, S., van Lanen, H. A. J., Looser, U., Prudhomme, C., Rees, G., Stahl, K., and Tallaksen, L. M.: Large-scale river flow archives: importance, current status and future needs, *Hydrol Process*, 25, 1191–1200, <https://doi.org/10.1002/HYP.7794>, 2011.

585

Hardenbicker, P., Viergutz, C., Becker, A., Kirchesch, V., Nilson, E., and Fischer, H.: Water temperature increases in the river Rhine in response to climate change, *Reg Environ Change*, 17, 299–308, <https://doi.org/10.1007/s10113-016-1006-3>, 2017.

590 Hochreiter, S. and Schmidhuber, J.: Long Short-Term Memory, *Neural Comput*, 9, 1735–1780, <https://doi.org/10.1162/NECO.1997.9.8.1735>, 1997.

595 Johnson, M. F., Albertson, L. K., Algar, A. C., Dugdale, S. J., Edwards, P., England, J., Gibbins, C., Kazama, S., Komori, D., MacColl, A. D. C., Scholl, E. A., Wilby, R. L., de Oliveira Roque, F., and Wood, P. J.: Rising water temperature in rivers: Ecological impacts and future resilience, *Wiley Interdisciplinary Reviews: Water*, e1724, <https://doi.org/10.1002/WAT2.1724>, 2024.





Jolliffe, I. T. and Stephenson, D. B.: Forecast verification. A practitioner's guide in atmospheric science, 2nd ed., Wiley-Blackwell, UK, 2012.

600

Kelleher, C. A., Golden, H. E., and Archfield, S. A.: Monthly river temperature trends across the US confound annual changes, *Environmental Research Letters*, 16, 104006, <https://doi.org/10.1088/1748-9326/AC2289>, 2021.

Kraft, B., Schirmer, M., Aeberhard, W. H., Zappa, M., Seneviratne, S. I., and Gudmundsson, L.: CH-RUN: A data-driven spatially contiguous runoff monitoring product for Switzerland, *EGUsphere Preprint*, <https://doi.org/10.5194/egusphere-2024-993>, 2024.

605

Laio, F. and Tamea, S.: Verification tools for probabilistic forecasts of continuous hydrological variables, *Hydrol Earth Syst Sci*, 11, 1267–1277, <https://doi.org/10.5194/HESS-11-1267-2007>, 2007.

610

Li, L., Jamieson, K., DeSalvo, G., Rostamizadeh, A., and Talwalkar, A.: Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization, *Journal of Machine Learning Research*, 18, 1–52, 2018.

Lim, B., Arık, S., Loeff, N., and Pfister, T.: Temporal Fusion Transformers for interpretable multi-horizon time series forecasting, *Int J Forecast*, 37, 1748–1764, <https://doi.org/10.1016/J.IJFORECAST.2021.03.012>, 2021.

615

Little, A. G., Loughland, I., and Seebacher, F.: What do warming waters mean for fish physiology and fisheries?, *J Fish Biol*, 97, 328–340, <https://doi.org/10.1111/JFB.14402>, 2020.

620 Meinshausen, N.: Quantile Regression Forests, *Journal of Machine Learning Research*, 7, 983–999, 2006.

Michel, A., Brauchli, T., Lehning, M., Schaepli, B., and Huwald, H.: Stream temperature and discharge evolution in Switzerland over the last 50 years: annual and seasonal behaviour, *Hydrol Earth Syst Sci*, 24, 115–142, <https://doi.org/10.5194/HESS-24-115-2020>, 2020.

625

Michel, A., Schaepli, B., Wever, N., Zekollari, H., Lehning, M., and Huwald, H.: Future water temperature of rivers in Switzerland under climate change investigated with physics-based models, *Hydrol Earth Syst Sci*, 26, 1063–1087, <https://doi.org/10.5194/HESS-26-1063-2022>, 2022.

630 Ouarda, T. B. M. J., Charron, C., and St-Hilaire, A.: Regional estimation of river water temperature at ungauged locations, *J Hydrol X*, 17, 100133, <https://doi.org/10.1016/J.HYDROA.2022.100133>, 2022.



Ouellet, V., St-Hilaire, A., Dugdale, S. J., Hannah, D. M., Krause, S., and Proulx-Ouellet, S.: River temperature research and practice: Recent challenges and emerging opportunities for managing thermal habitat conditions in stream ecosystems, *Science of The Total Environment*, 736, 139679, <https://doi.org/10.1016/J.SCITOTENV.2020.139679>, 2020.

Ouellet-Proulx, S., St-Hilaire, A., and Boucher, M. A.: Water Temperature Ensemble Forecasts: Implementation Using the CEQUEAU Model on Two Contrasted River Systems, *Water* 2017, Vol. 9, Page 457, 9, 457, <https://doi.org/10.3390/W9070457>, 2017.

640

Qiu, R., Wang, Y., Rhoads, B., Wang, D., Qiu, W., Tao, Y., and Wu, J.: River water temperature forecasting using a deep learning method, *J Hydrol (Amst)*, 595, 126016, <https://doi.org/10.1016/J.JHYDROL.2021.126016>, 2021.

Singh, G. G., Sajid, Z., and Mather, C.: Quantitative analysis of mass mortality events in salmon aquaculture shows increasing scale of fish loss events around the world, *Scientific Reports* 2024 14:1, 14, 1–10, <https://doi.org/10.1038/s41598-024-54033-9>, 2024.

Toffolon, M. and Piccolroaz, S.: A hybrid model for river water temperature as a function of air temperature and discharge, *Environmental Research Letters*, 10, 114011, <https://doi.org/10.1088/1748-9326/10/11/114011>, 2015.

650

Tripathy, K. P. and Mishra, A. K.: Deep learning in hydrology and water resources disciplines: concepts, methods, applications, and research directions, *J Hydrol (Amst)*, 130458, <https://doi.org/10.1016/J.JHYDROL.2023.130458>, 2023.

van Vliet, M. T. H., Franssen, W. H. P., Yearsley, J. R., Ludwig, F., Haddeland, I., Lettenmaier, D. P., and Kabat, P.: Global river discharge and water temperature under climate change, *Global Environmental Change*, 23, 450–464, <https://doi.org/10.1016/J.GLOENVCHA.2012.11.002>, 2013.

van Vliet, M. T. H., Florke, M., and Wada, Y.: Quality matters for water scarcity, *Nature Geoscience* 2017 10:11, 10, 800–802, <https://doi.org/10.1038/ngeo3047>, 2017.

660

van Vliet, M. T. H., Thorslund, J., Stokal, M., Hofstra, N., Flörke, M., Ehalt Macedo, H., Nkwasa, A., Tang, T., Kaushal, S. S., Kumar, R., van Griensven, A., Bouwman, L., and Mosley, L. M.: Global river water quality under climate change and hydroclimatic extremes, *Nature Reviews Earth & Environment* 2023 4:10, 4, 687–702, <https://doi.org/10.1038/s43017-023-00472-3>, 2023.

665



Wade, J., Kelleher, C., and Hannah, D. M.: Machine learning unravels controls on river water temperature regime dynamics, *J Hydrol (Amst)*, 623, 129821, <https://doi.org/10.1016/J.JHYDROL.2023.129821>, 2023.

670 Webb, B. W.: Trends in stream and river temperature, *Hydrol Process*, 10, 205–226, [https://doi.org/10.1002/\(SICI\)1099-1085\(199602\)10:2<205::AID-HYP358>3.0.CO;2-1](https://doi.org/10.1002/(SICI)1099-1085(199602)10:2<205::AID-HYP358>3.0.CO;2-1), 1996.

Wen, R., Torkkola, K., Narayanaswamy, B., and Madeka, D.: A Multi-Horizon Quantile Recurrent Forecaster, 2018.

675 Wright, M. N. and Ziegler, A.: Ranger: A fast implementation of random forests for high dimensional data in C++ and R, *J Stat Softw*, 77, <https://doi.org/10.18637/JSS.V077.I01>, 2017.

Zhu, S. and Piotrowski, A. P.: River/stream water temperature forecasting using artificial intelligence models: a systematic review, *Acta Geophysica*, 68, 1433–1442, <https://doi.org/10.1007/S11600-020-00480-7/TABLES/1>, 2020.