Evaluation of water flux predictive models developed using eddy covariance observations and machine learning: a meta-analysis

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Abstract.

With the rapid accumulation of water flux observations from global eddy-covariance flux sites, many studies have used data-driven approaches to model site-scale water fluxes with various predictors and machine learning algorithms used. However, systematic evaluation of such models is still limited. We therefore performed a meta-analysis of 32 such studies, derived 139 model records, and evaluated the impact of various features on model accuracy throughout the modeling flow. SVM (average R-squared = 0.82) and RF (average R-squared = 0.81) outperformed over evaluated algorithms with sufficient sample size in both cross-study and intra-study (with the same ~~training dataset~~data) comparisons. The average accuracy of the model applied to arid regions is higher than in other climate ~~classes~~types. The average accuracy of the model was slightly lower for forest sites (average R-squared = 0.76) than for ~~cropland~~croplands and ~~grassland sites~~grasslands (average R-squared = 0.8 and 0.79), but higher than for ~~shrub~~shrubland sites (average R-squared = 0.67). ~~Among various predictor variables, the use of net/sun radiation~~Using Rn/Rs, precipitation, ~~air temperature~~Ta, and ~~the fraction of absorbed photosynthetically active radiation~~FAPAR improved the model accuracy. ~~Among the different validation methods, random~~The combined use of Ta and Rn/Rs is very effective especially in forests, while in grasslands the combination of Ws and Rn/Rs is also effective. Random cross-validation ~~shows~~showed higher model accuracy than spatial cross-validation and temporal cross-validation, but spatial cross-validation is more important ~~for the application for water flux predictive models when used for~~in spatial extrapolation. The findings of this study are promising to guide future research on such machine learning-based modeling.

1 Introduction

Evapotranspiration (ET) is one of the most important ~~indicator~~components of the water cycle in terrestrial ecosystems. It also represents the key variable in linking ecosystem functioning, carbon and climate feedbacks, agricultural management, and water resources (Fisher et al., 2017). The quantification of ET for regional, continents, or the globe can improve our understanding of the water, heat, and carbon interactions, which is important for global change research (Xu et al., 2018). Information on ET has been used in many fields, including, but not limited to, droughts and heatwaves (Miralles et al., 2014), regional water balance closures (Chen et al., 2014; Sahoo et al., 2011), agricultural management (Allen et al., 2011), water resources management (Anderson et al., 2012), biodiversity patterns (Gaston, 2000). In addition, accurate large-scale and long-time series ET prediction at high spatial and temporal resolution has been of great interest (Fisher et al., 2017).

Currently, there are three main approaches for simulation and spatial and temporal prediction of ET: (i) physical models based on remote sensing such as surface energy balance models (Minacapilli et al., 2009; Wagle et al., 2017), Penman-Monteith equation (Mu et al., 2011; Zhang et al., 2010), Priestley-Taylor equation (Miralles et al., 2011); (ii) process-based land surface models, biogeochemical models and hydrological models (Barman et al., 2014; Pan et al., 2015; Sándor et al., 2016; Chen et al., 2019); and (iii) the observation-based machine learning modeling approach with in situ eddy covariance (EC) observations of water flux ~~(Jung et al., 2011; Li et al., 2018; Van Wijk and Bouten, 1999; Xie et al., 2021; Xu et al., 2018; Yang et al., 2006; Zhang et al., 2021)~~. ~~For remote sensing-based physical models and process-based land surface models, some physical processes~~

~~have not been well characterized due to the lack of understanding of the detailed mechanisms influencing ET under different environmental conditions.~~(Jung et al., 2011; Li et al., 2018; Van Wijk and Bouten, 1999; Xie et al., 2021; Xu et al., 2018; Yang et al., 2006; Zhang et al., 2021). For remote sensing-based physical models and process-based land surface models, some physical processes have not been well characterized due to the lack of understanding of the detailed mechanisms influencing ET under different environmental conditions. For example, the inaccurate representation and estimation of stomatal conductance (Li et al., 2019) and the linearization (McColl, 2020) of the Clausius-Clapeyron relation in the Penman-Monteith equation may introduce both empirical and conceptual errors into estimates of ET. Limited by complicated assumptions and model parametrizations, these process-based models face challenges in the accuracy of their ET estimations over heterogeneous landscapes (Pan et al., 2020; Zhang et al., 2021). Therefore, many researchers have used data-driven approaches for the simulation and prediction of ET with the accumulation of a large volume of measured site-scale observational data of water fluxes in the past decades. Various machine learning models have been developed to simulate water fluxes at the flux site scale. Besides, various predictor variables (e.g., meteorological factors, vegetation conditions, and moisture supply conditions) have been incorporated into such models for upscaling (Fang et al., 2020; Jung et al., 2009) of water flux to a larger scale or understanding the driving mechanisms with the variable importance analysis performed in such models.

However, to date, the systematic assessment of the uncertainty in the processes of water flux prediction models constructed using the machine learning approach is limited. Although considerable effort has been invested in improving the accuracy of such prediction models, our understanding of the expected accuracy of such models under different conditions is still limited. It is still not easy for us to give the general guidelines for selecting appropriate predictor variables and models. Questions such as 'Which predictor variables are the best in water flux simulations?' and 'How to improve the prediction accuracy of water flux effectively?' etc. still confuse the researchers in the field. Therefore, we should synthesize the findings from published ~~such~~ studies to determine which predictor variables, machine learning models, and other features can significantly improve the prediction accuracy of water flux. Also, we are interested in understanding under which specific conditions they are more effective.

A variety of features ~~may affect~~control the accuracy of such models, including the predictor variables used, the inherent heterogeneity within the dataset, the plant functional type (PFT) of the flux sites, the method of model construction and validation, and the ~~machine learning~~ algorithm chosen:

a) Predictor variables used: Compared to process-based models, the data used may have a more significant impact on the final model performance in data-driven models. Various biophysical covariates and other environmental factors have been used for the simulation and prediction of water fluxes. The most commonly used factors include mainly precipitation (Prec), air temperature (Ta), wind speed (Ws), net/sun radiation (Rn/Rs), soil temperature (Ts), soil texture, vapor-pressure deficit (VPD), the fraction of absorbed photosynthetically active radiation (FAPAR), vegetation index (e.g., Normalized Difference Vegetation Index (NDVI~~,~~), Enhanced Vegetation Index (EVI~~),~~)), Leaf area index (LAI~~,~~), and carbon fluxes (e.g., Gross Primary Productivity (GPP~~).~~)). These used predictor variables and their complex interactions drive the fluctuations and variability of water fluxes. They affect the accuracy of water flux simulations in two ways: their actual impact on water fluxes at the process-based level and their spatio-temporal resolution and inherent accuracy. The relationship between water fluxes and these variables at the process-based driving mechanism level is very different under different PFTs, different climate types, and different hydrometeorological conditions. For example, in irrigated croplands in arid regions, water fluxes may be highly correlated with irrigation practices, and thus soil moisture may be a very important predictor variable, and its importance may be significantly higher than in other PFTs. And in models that incorporate data from multiple PFTs, some variables that play important roles in multiple PFTs may have higher importance. In terms of data spatial and temporal resolution, the data for these predictor variables may have different scales. In terms of spatial resolution, meteorological observations such as precipitation and air temperature are at the flux site scale, while factors extracted from satellite remote sensing and reanalysis climate datasets cover a much larger spatial scale (i.e. the grid-scale). This leads to considerable differences in the degree of spatial match between different variables and the site scale EC observations (approximately 100 m x 100 m). It is therefore difficult for some variables to be fairly compared in the subsequent importance analysis of driving factors. In terms of temporal resolution, the importance of predictor variables with different temporal resolutions may be variable for models with different time scales (e.g., half-hourly, daily, and monthly models). For example, the daily or 8-day NDVI data based on MODIS satellite imagery may better capture the temporal dynamics of water fluxes concerning vegetation growth than the 16-daily NDVI data derived from Landsat images. Besides, data on non-temporal dynamic variables such as soil texture cannot explain temporal variability in water fluxes in the data-driven simulations, although soil texture may be important in the interpretation of the actual driving mechanisms of ET (which may need to be quantified in detail in ET simulations by process-based models). In addition, some inherent accuracy issues (e.g., remote sensing-based NDVI may not be effective at high values) of the predictors may propagate into the consequent machine learning models, thus affecting the modeling and our understanding of its importance. Therefore, it is necessary to consider the spatial and temporal resolution of the data and their inherent accuracy for the predictors used in different studies in the systematic evaluation of data-driven water flux simulations.

b) The ~~volume of the dataset, inherent~~ heterogeneity of the dataset~~,~~ and ~~how the~~ model ~~is validated~~validation: the volume and inherent spatiotemporal heterogeneity of the training dataset (with more variability and extremes incorporated) may affect model accuracy. Typically, training data with larger regions, multiple sites, multiple PFTs, and longer year spans may have a higher degree of imbalance ~~(Kaur et al., 2019; Van Hulse et al., 2007; Virkkala et al., 2021; Zeng et al., 2020)~~(Kaur et al., 2019; Van Hulse et al., 2007; Virkkala et al., 2021; Zeng et al., 2020). And in machine learning, in general, modeling with unbalanced data (with significant differences in the distribution between the training and validation sets) may result in lower model accuracy. Currently, the most common ways of model validation include spatial, temporal, and random cross-validation. Spatial validation is mainly to evaluate the ability of the model to be applied in different regions or flux sites with different PFT types, and one of the common methods is 'leave one site out' (Fang et al., 2020; Papale et al., 2015; Zhang et al., 2021). If the data of the site left out for validation differs significantly from the distribution of the training data set, the expected accuracy of the model applied at that site may be low because the trained model may not capture the specific and local relationships between the water flux and the various predictor variables at that site. For temporal validation, to assess the ability of the models to adapt to the interannual variability, typically some years of data are used for training and the remaining years for model validation (Lu and Zhuang, 2010). If a year with extreme climate is used for validation, the accuracy may be low because the training dataset may not contain such extreme climate conditions. In the case of PFTs that are significantly affected by human activities, such as cropland, the possible different crops grown and different land use practices (e.g., irrigation) across years can also lead to low accuracy in temporal validation. ~~K-fold cross-validation is commonly used in random cross-validation to assess the fitness of the model to the spatio-temporal variability. In this case, different values of K may also affect the model accuracy. For example, for an unbalanced dataset, the average model accuracy obtained from a 10-fold (K = 10) validation approach is likely to be higher than that of a 3-fold (K = 3) validation approach.~~

c) Various machine learning algorithms: Some machine learning algorithms may have specific advantages when applied to model the relationships between water fluxes and covariates. For example, neural networks may have an advantage in nonlinear fitting, while random forests ~~may~~can avoid serious overfitting ~~due to the introduction of randomness~~problems. However, which algorithm is better overall in different situations (i.e. applied to different data sets)? Which algorithm is generally more accurate than the others when using the same data set? A comprehensive evaluation ~~of this~~ is ~~necessary.~~ important.

Therefore, to systematically and comprehensively assess the impact of various features in such modeling, we perform a meta-analysis of published water flux simulation studies that combine the flux site water flux observations, various predictors, and machine learning. The accuracy of model records collected from the literature was linked with various model features to assess the impacts of predictor data types, algorithms, and other features on model accuracy. The findings of this study may be promising to improve our understanding of the impact of various features of the models to guide future research on such machine learning-based modeling.

2 Methodology

2.1 Protocol for selecting the sample of articles

We applied a general query (on December 1st, 2021) on title, abstract, and keywords to include articles with the "OR" operator applied among expressions (Table 1) in the Scopus database. Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) (Moher et al., 2009) ~~is~~are followed when filtering the papers. We first excluded articles that obviously did not fit the topic of this study based on the abstract, and then performed the article screening with the full-text reading.

The inclusion of articles follows the following criteria:

a) Articles were filtered for those with water fluxes (or latent heat) simulated~~, with multi-variable~~.

b) The water flux or latent heat observations used in the prediction models should be from the eddy-covariance flux measurements.

c) Articles focusing only on gap-filling (Hui et al., 2004) techniques (i.e., the objective was not simulation and extrapolation of water fluxes using machine learning) were excluded.

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d) Only articles that used multivariate regression ~~used, (~~with the number of covariates greater than or equal to 3) were included.

e) The determination coefficient (R-squared) of the validation step should be reported as the metric of model performance ~~(Shi et al., 2021; Tramontana et al., 2016; Zeng et al., 2020), and published in English journals.~~ (Shi et al., 2021; Tramontana et al., 2016; Zeng et al., 2020) in the articles.

f) The articles should be published in English-language journals.

Although RMSE is also often used for model accuracy assessment, its dependence on the magnitude of water flux values makes it difficult to use for fair comparisons between studies. For example, due to the difference in the range of ET values, models developed from flux stations in dry grasslands will typically have lower RMSE than models developed by flux stations based on forests in humid regions. Therefore, RMSE may not be a good metric for cross-study comparisons in this meta-analysis.

Table 1. Article search: '[A1 OR A2 OR A3...] AND [B1 OR B2 OR B3...] AND [C1 OR C2 OR C3 OR C4...]'

ID	A	B	C
1	Water flux	Eddy covariance	Machine learning
2	Evapotranspiration	Flux tower	Support Vector
3	Latent heat	Flux site	Neural Network
4			Random Forest

2.2 Features of the prediction processes evaluated

The various features (Table 2) involved in the water flux modeling framework (Fig. 1) include the PFTs of the sites, the predictors used, the machine learning algorithms, the validation methods, and other features. Each model for which R-squared is reported is treated as a data record. If multiple algorithms were applied to the same dataset, then multiple records were extracted. Models using different data or features are also recorded as multiple records.

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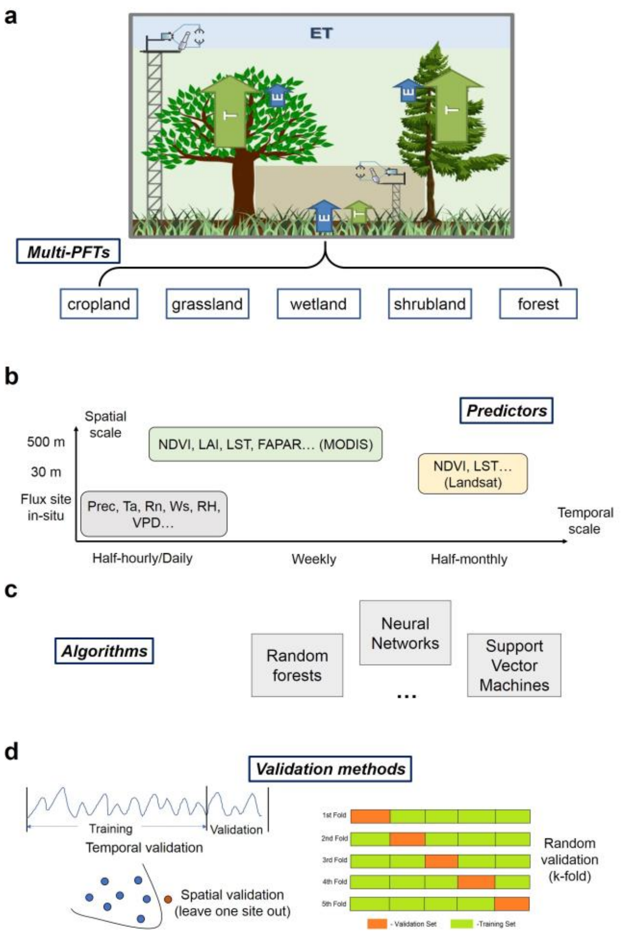

Figure 1. Features of the machine learning-based water flux prediction process. (a) the eddy-covariance-based water flux observations of various plant function types (PFTs), modified from Paul-Limoges et al., 2020. ET, evapotranspiration. E, evaporation. T, transpiration. (b) Predictors and their spatial and temporal resolution. (c) The machine learning algorithms used for the modeling, such as neural networks, random forests, etc. (d) The model validation methods used including the spatial, temporal, and random cross-validations.

Table 2. Description of information extracted from the included papers.

Field~~Feature~~	**Definition & Categories adopted**	**~~Categories adopted~~Harmonization**
Climate	Climate ~~zone~~zones of the study location derived from the Köppen climate classification (Peel et al., 2007)	
Plant functional type (PFT)	PFT of the flux sites: 1-forest, 2-grassland, 3-cropland, 4-wetland, 5-shrubland, 6-savannah, and multi-PFTs	~~1-forest, 2-grassland, 3-cropland, 4-wetland, 5-shrubland, 6-savannah, and multi-PFTs~~The categorization is based on

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		the descriptions in the article. For example, cropland for various crops is classified as 'cropland', and both woody savannah and savannah are classified as 'savannah'.
Location	More precise location (with the latitude and longitude of the center of the studied sites~~).~~): latitude, longitude	~~latitude, longitude~~
Algorithms	Random Forests (RF), Multiple Linear Regressions (MLR), Artificial Neural Networks (ANN), Support Vector Machines (SVM), Cubist, model tree ensembles (MTE), K-nearest neighbors (KNN), long short-term memory (LSTM), gradient boosting regression tree (GBRT), extra tree regressor (ETR), Gaussian process regression (GPR), Bayesian model averaging (BMA), extreme learning machine (ELM), and deep belief network (DBN)~~Algorithm families used~~	Various model algorithms with parameter optimization or other improvements are categorized as their algorithm family. For example, various improved models of RF algorithms are classified as RF, rather than as another algorithm family.~~Random Forests (RF), Multiple Linear Regressions (MLR), Artificial Neural Networks (ANN), Support Vector Machines (SVM), Cubist, model tree ensembles (MTE), K-nearest neighbors (KNN), long short-term memory (LSTM), gradient boosting regression tree (GBRT), extra tree regressor (ETR), Gaussian process regression (GPR), Bayesian model averaging (BMA), extreme learning machine (ELM), and deep belief network (DBN)~~
Sites number	Number of the flux sites used	
Spatial scale	Area representatively covered by the flux sites: local (less than 100 x 100 km), regional, global (continent-scale and global scale)	~~local (less than 100 x 100 km), regional, global (continent-scale and global scale)~~The spatial scale is roughly categorized based on the area covered by the site. The model is classified as 'global' only when the spatial extent reaches the continental scale.
Temporal scale	The temporal scale of the model: half-hourly, hourly, daily, 4-daily, 8-daily, monthly, seasonally (i.e., 0.02, 0.04, 1, 4, 8, 30, 90 days)	~~half-hourly, hourly, daily, 4-daily, 8-daily, monthly, seasonally (i.e., 0.02, 0.04, 1, 4, 8, 30, 90 days)~~Models with a temporal scale greater than one month and less than one year are classified as seasonal scale models.
Year span	The span of years of the flux data used	Year span is calculated as the span from the earliest to the latest year of available flux data.
Site year	Describe the volume of total flux data with the number of sites and years aggregated.	
Cross-validation	Describe the chosen method of cross-validation: Spatial (e.g., 'leave one site out'), temporal (e.g., 'leave one year out'), random (e.g., 'k-fold')~~.~~	~~Spatial (e.g., 'leave one site out'), temporal (e.g., 'leave one year out'), random (e.g., 'k-fold')~~
Training/validation	Describe the ratio of the data volume in the training and validation sets.	In spatial validation, this ratio is represented by the ratio of the number of sites used for training to the number of sites used for validation. In temporal validation, this is represented by the ratio of the span of time periods used for

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		training to the span of time periods used for validation.
Satellite images	Describe the source of satellite images used to derive NDVI, EVI, LAI, LST, etc~~.~~: Landsat, MODIS, AVHRR	~~Landsat, MODIS, AVHRR~~
Biophysical predictors	LAI, NDVI/EVI,~~ enhanced vegetation index (EVI),~~ the fraction of absorbed photosynthetically active radiation/photosynthetically active radiation (FAPAR/PAR), leaf area index (LAI), Carbon fluxes (CF) including NEE/GPP, etc.	~~Used (recorded as '1') or not used (recorded as '0')~~The predictor variables of different measurement methods are categorized according to their definitions. For example, both using the NDVI calculated based on satellite remote sensing bands and in situ measurements were classified as the use of 'NDVI'.
Meteorological variables	precipitation (Prec), net radiation/solar radiation (Rn/Rs), air temperature (Ta), vapour-pressure deficit (VPD), relative humidity (RH) , etc.	~~Used (recorded as '1') or not used (recorded as '0')~~The way meteorological data are measured is not differentiated. For example, both using Ta from reanalysis data and Ta measured at flux sites were classified as the use of Ta.
Ancillary data	Describe the ancillary variables used: soil texture, terrain (DEM), soil moisture/land surface water index (SM/LSWI), etc.	~~Used (recorded as '1') or not used (recorded as '0')~~Both the use of in situ measured soil moisture and the use of remote sensing-based LSWI was classified as using surface moisture-related indicators SM/LSWI.
~~Top three variables in the ranking of importance of predictors~~	~~Describe the interpretation of the importance of variables reported in the machine learning models.~~	
Accuracy measure	Accuracy measure used to assess the model performance: R-squared (in the validation phase)	~~R-squared (in the validation phase)~~

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3 Results

3.1 Articles included in the meta-analysis

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A total of 32 articles (~~see Supplement Information~~Table S1) containing a total of 139 model records were included. The geographical scope of these articles was mainly Europe, North America, and China (Fig. 2).

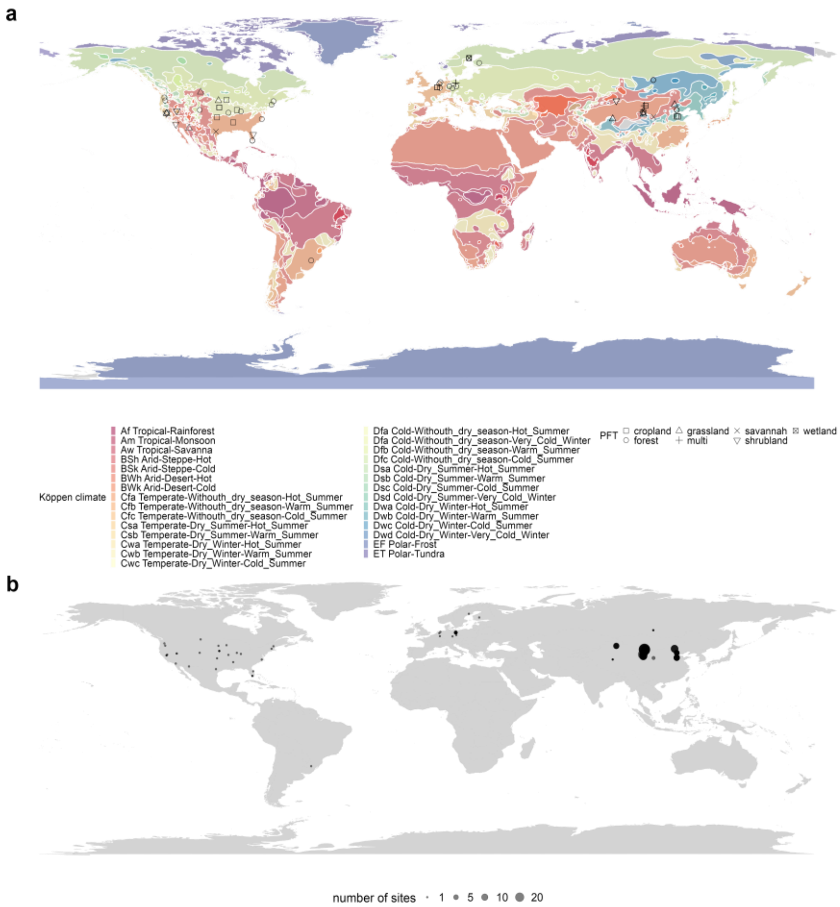

Figure 2. Location of the included studies in the meta-analysis. (a) PFTs and the climate zones (from Köppen climate classification) of these studies and (b) the number of flux sites included in each study. Global and continental-scale studies (e.g., models developed based on FLUXNET of the global scale) are not shown on the map due to the difficulty of identifying specific locations.

3.2 The formal Meta-analysis

~~We formally assessed the impact of the features (e.g., algorithms, study area, PFTs, the volume of data used, validation methods, predictor variables, etc.) used in the different models based on differences of R-squared.~~

3.2.1 Algorithms

SVM and RF outperformed (Fig. 3a) across studies (~~lightly~~ better than other algorithms with sufficient sample size in Fig. 3a such as ANN). These three machine learning algorithms (i.e., ANN, SVM, RF) were significantly more accurate than the traditional MLR. Other algorithms such as MTE, ELM, Cubist, etc. also correspond to

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high accuracy, but with limited evidence sample size~~.~~ (Fig. 3a). In the internal comparison (different algorithms applied to the same data set) in single studies, we also find that SVM and RF were ~~significantly~~slightly more accurate than ANN (Fig. 3b), and all these three (i.e., ANN, SVM, RF) are ~~significantly~~considerably more accurate than MLR. Overall, SVM and RF have shown higher accuracy in water flux simulations~~.~~ in both inter and intra-study comparisons with sufficient sample size as evidence.

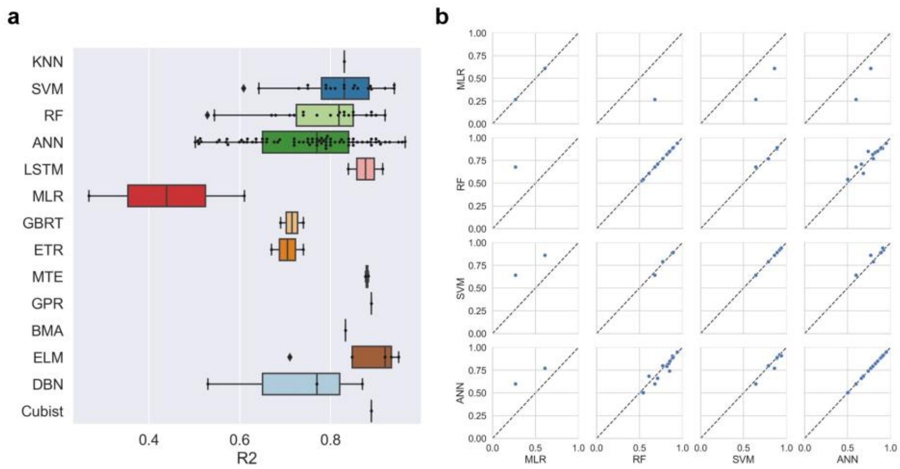

Figure 3. ~~Differences in model~~Model accuracy (R-squared) using ~~different~~various algorithms across studies (a) and internal comparisons of ~~the model accuracy (R-squared) of~~ selected pairs of algorithms within ~~individual~~ studies (b). ~~Regression algorithms~~Algorithms: Random Forests (RF), Multiple Linear Regressions (MLR), Artificial Neural Networks (ANN), Support Vector Machines (SVM), Bayesian model averaging (BMA), Cubist, model tree ensembles (MTE), ~~K-nearest neighbors (KNN), long short-term memory (LSTM),~~ gradient boosting regression tree (GBRT), extra tree regressor (ETR), K-nearest neighbors (KNN), long short-term memory (LSTM), Gaussian process regression (GPR), ~~Bayesian model averaging (BMA),~~ extreme learning machine (ELM), and deep belief network (DBN).

3.2.2 Climate types and PFTs

We found higher average model accuracy in arid climate zones (Fig. 4a), such as the Cold semi-arid (steppe) climate (BSk) and Cold desert climate (BWk~~.~~). Most of these studies were located in northwest China and the western USA. It may be caused by the simpler relationship between water fluxes and biophysical covariates in arid regions. In arid zones, due to the high potential ET, the variability in the actual ET may be largely explained by water availability (moisture supply) and vegetation change with the effect of variability in thermal conditions reduced. As for the various PFTs, the average model accuracy was slightly lower for forest types than for cropland and grassland types (Fig. ~~4b) possibly because some remote sensing-based predictors such as FAPAR and LAI have limited accuracy when applied to forest types (Fig. 5). The lowest average accuracy was found for shrub sites, which may be related to the difficulty of remote sensing-based NDVI, etc., to quantify the physiological and ecological conditions of shrubs,~~4b). The lowest average accuracy was found for shrub sites, which may be related to the difficulty of the remote sensing-based vegetation index (e.g., NDVI) to quantify the physiological and ecological conditions of shrubs (Zeng et al., 2022), and the heterogeneity of the spatial distribution of shrubs within the EC observation area may also cause difficulties in capturing their relationships with biophysical variables. We also found high model accuracy for the wetland type, although records as evidence to support this finding may be limited. Compared to other PFTs, the more steady and adequate water availability in the wetland type may make the variations of water fluxes less explained by other biophysical covariates.

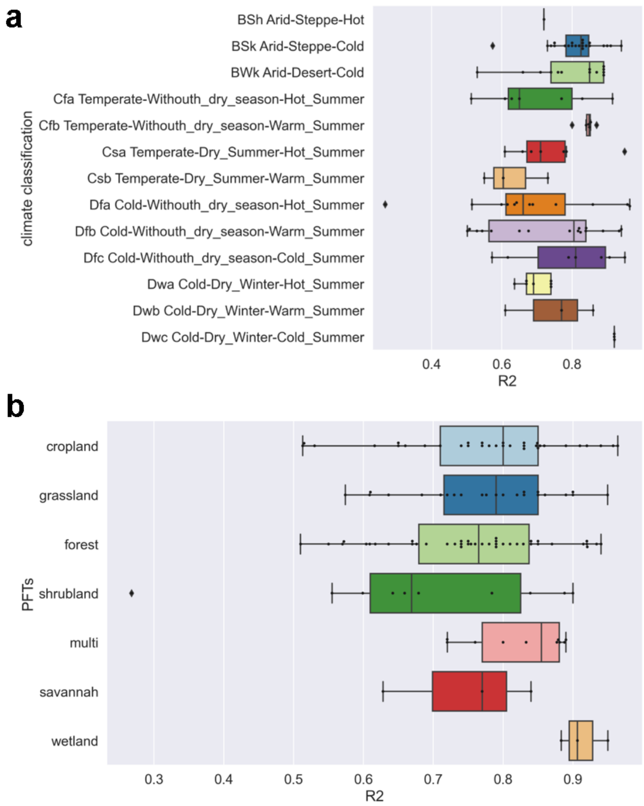

Figure 4. Differences in model accuracy (R-squared) of (a) various climate zones (classified by Köppen climate classification) across studies and (b) PFTs. BSh, Hot semi-arid (steppe) climate. BSk, Cold semi-arid (steppe) climate. BWk, Cold desert climate. Cfa, Humid subtropical climate. Cfb, Temperate oceanic climate. Csa, Hot-summer Mediterranean climate. Csb, Warm-summer Mediterranean climate. Dfa, Hot-summer humid continental climate. Dfb, Warm-summer humid continental climate. Dfc, Subarctic climate. Dwa, Monsoon-influenced hot-summer humid continental climate. Dwb, Monsoon-influenced warm-summer humid continental climate. Dwc, Monsoon-influenced subarctic climate.

~~Among~~3.3.3 Predictors and their combinations

On one hand, for the ~~various~~effects of individual predictors, the use of Rn/Rs, Prec, Ta, and FAPAR ~~significantly~~ improved the accuracy of the model (Fig. ~~5~~S1). This pattern partially changed in the different PFTs. In the forest sites, the accuracy of the models with Rn/Rs and Ta used was ~~significantly~~ higher than that of the models with Rn/Rs and Ta not used. For the grassland sites, the use of Ws, FAPAR, Prec, and Rn/Rs ~~significantly~~ improved the model accuracy. For the cropland sites, Ta and FAPAR were more important for improving the model accuracy.

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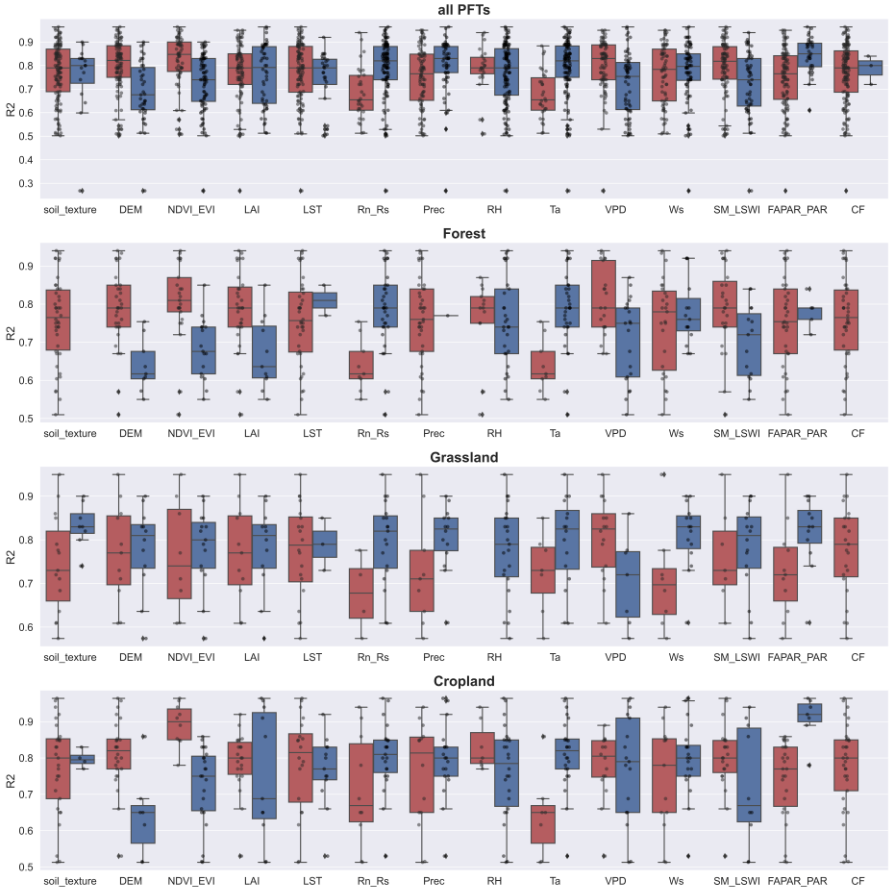


~~Figure 5. The impact of the various predictors used in models of different PFTs (all data, forest, grassland, and cropland) on R-squared. Dark blue boxes indicate that the predictor was used in the model, while dark red boxes indicate that the predictor was not used. Predictors: precipitation (Prec), soil moisture/land surface water index (SM_LSWI), net radiation/solar radiation (Rn_Rs), enhanced vegetation index (EVI), air temperature (Ta), vapor-pressure deficit (VPD), the fraction of absorbed photosynthetically active radiation/photosynthetically active radiation (FAPAR_PAR), relative humidity (RH), carbon flux (CF), leaf area index (LAI).~~

On the other hand, the evaluation of the effect of individual predictors on model accuracy is not necessarily reliable because some predictor variables are used together (e.g., the high model accuracy corresponding to a particular variable may be because it is often used together with another variable that plays the dominant role in improving accuracy). Therefore, we tested for independence between the use of variables and assessed the effect of the combination of variables on model accuracy. We calculated the correlation matrix (Fig. S2) between the use of various predictors (not used is set as 0 and used is set as 1). We found there was a dependence between the use of some predictors, the use of NDVI/EVI, LAI, and SM was significantly negatively correlated with the use of Rn/Rs and Ta (Fig. S2). It indicated that many of the models that used Rn/Rs and Ta did not use NDVI/EVI, LAI, and SM, and the models that used NDVI/EVI, LAI, and SM also happened to not use Rn/Rs and Ta. Given this dependence, we evaluated the effect of the combination of variables on the model accuracy (Fig. 5). In Fig. 5, the three variable combinations on the left side are mainly meteorological variables while the three variable combinations on the right side are mainly vegetation-related variables based on remote sensing (e.g., NDVI, EVI, LAI, LSWI). We found that, overall, the accuracy of the models using only meteorological variable combinations was higher than that of the models using only remote sensing-based vegetation-related variables. It demonstrated the importance of using meteorological variables in machine learning-based ET prediction (probably especially for models with small time scales such as hourly scale, and daily scale). For example, in the forest type, the combination of Ta and Rn/Rs is very effective compared to using only remote sensing-based vegetation index variable combinations. The combination of Ta and Rn/Rs is also effective in the grassland and cropland types. The combination of Ws and Rn/Rs played an important role in the grassland type for improving model accuracy. Despite this, it does not negate the positive role of remote sensing-based vegetation-related variables in ET prediction. This effectiveness can be dependent on the time scale of the model as well as the PFTs. In models with large time scales (monthly scale, seasonal scale) and PFTs in which ET is sensitive to vegetation dynamics, remote sensing-based vegetation-related variables may also be of high importance.

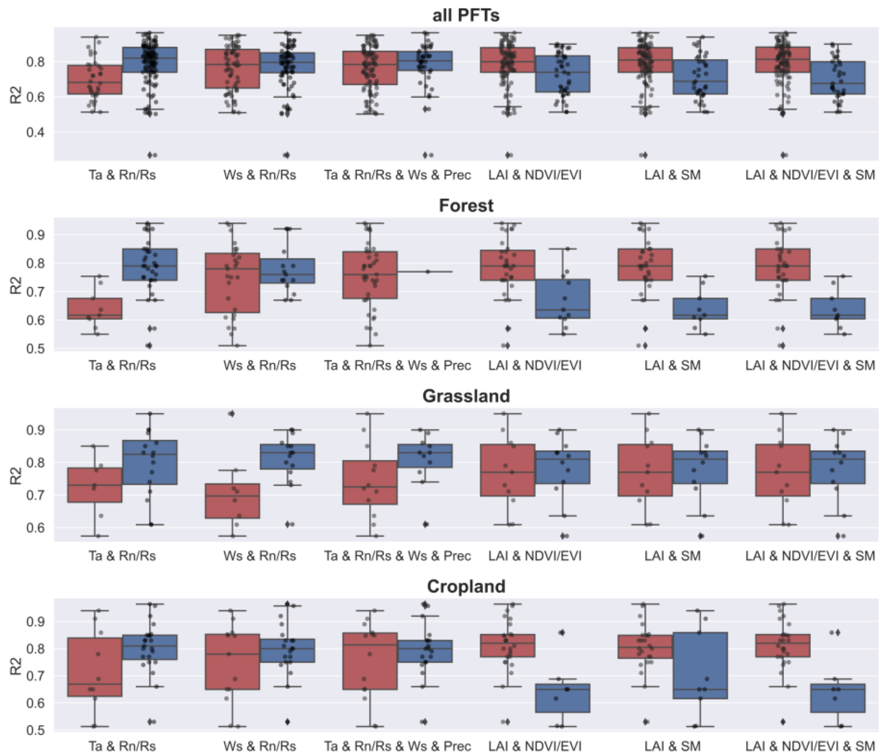
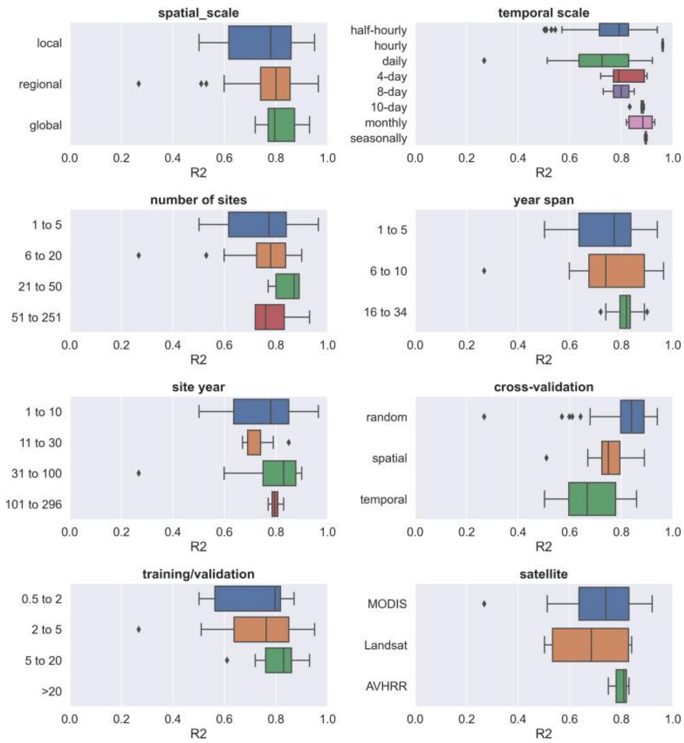


Figure 5. Effects of combinations of predictor variables on model accuracy in various PFTs (all data, forest, grassland, and cropland). Dark blue boxes indicate that the predictors were together used in the model (e.g., for 'Ta & Rn/Rs', the dark blue box represents Ta and Rn/Rs were together used in the model), while dark red boxes indicate the other conditions (i.e., the combination was not used). Predictors: precipitation (Prec), soil moisture/remote sensing-based land surface water index (SM), net radiation/solar radiation (Rn/Rs), enhanced vegetation index (EVI), air temperature (Ta), leaf area index (LAI), Normalized Difference Vegetation Index/Enhanced Vegetation Index (NDVI/EVI).

3.3.4 Other model features

We also evaluated the impact of some other features on accuracy. The differences in accuracy of models with different spatial scales, year spans, number of sites, and volume of data (Fig. 6) appear to be insignificant. This seems to be related to the fact that in large~~–~~scale water flux simulations, the sites of similar PFTs are selected such as for modeling multiple forest sites across Europe (Van Wijk and Bouten, 1999) which focus on 'forest' and multiple grassland sites across arid northern China (Xie et al., 2021; Zhang et al., 2021) which focus on 'grassland', rather than mixing different PFT types to train models as the way in machine learning modeling of carbon fluxes ~~(Zeng et al., 2020)~~(Zeng et al., 2020). In terms of the time scales of the models, the 4-day, 8-day, and monthly scales appear to correspond to higher accuracy compared to the half-hourly and daily scales. ~~Also,~~

~~the variability of the accuracy of the half-hourly and daily scale models is higher.~~ The higher the ratio of the volume of data in the training and validation sets, the higher the model accuracy. Compared to the models using Landsat data, the models using MODIS data showed slightly higher accuracy probably due to the advantage of MODIS data in capturing the temporal dynamics of biophysical covariates. There were significant differences in the accuracy of the models using different cross-validation methods, with the models using random cross-validation showing higher accuracy than those using temporal cross-validation. This suggests that interannual variability may have a high impact on the models in water flux simulations. The driving mechanism of ET may vary significantly across years, and the inclusion of some extreme climatic conditions in the training set may be important for model accuracy and robustness.



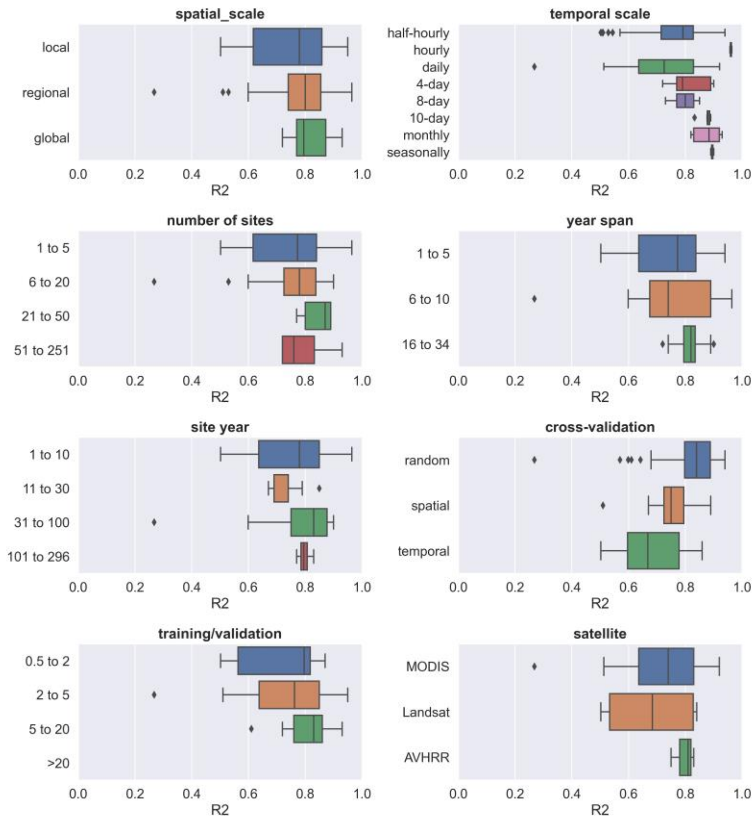


Figure 6. The ~~impacts~~effects of other model features (i.e. spatial scale, ~~temporal scale,~~ number of sites, temporal scale, year span, site year, ~~cross-~~validation method, training/validation ratio, and satellite imagery used) on the ~~model performance.~~ R-squared.

3.3.5 Linear correlation of quantitative features and R-squared

We also analyzed the linear correlation (Fig. 7) between multiple quantitative features and the R-squared. We found that the magnitude of the linear correlation coefficients between the use of predictor combinations and the R-squared was higher than other features. The use of the predictor combination ‘Ta and Rn/Rs’ significantly improved the model accuracy. ‘Temporal scale’, ‘time span’, ‘training/validation ratio’, and ‘number of sites’ showed weak positive correlations with R-squared (not significant, p-value > 0.1). The positive correlation between ‘temporal scale’ and R-squared is higher among these features, although not significant. It should also be paid more attention to in future studies. The feature 'training/validation ratio' and 'time span' are also positively correlated (although not significantly) with the R-squared, suggesting the importance of the volume of data in the training set in a data-driven machine learning model. Larger 'training/validation ratio' and 'time span' may correspond to greater proportional coverage of the scenarios/conditions in the training set over the validation set, and thus correspond to higher accuracy.

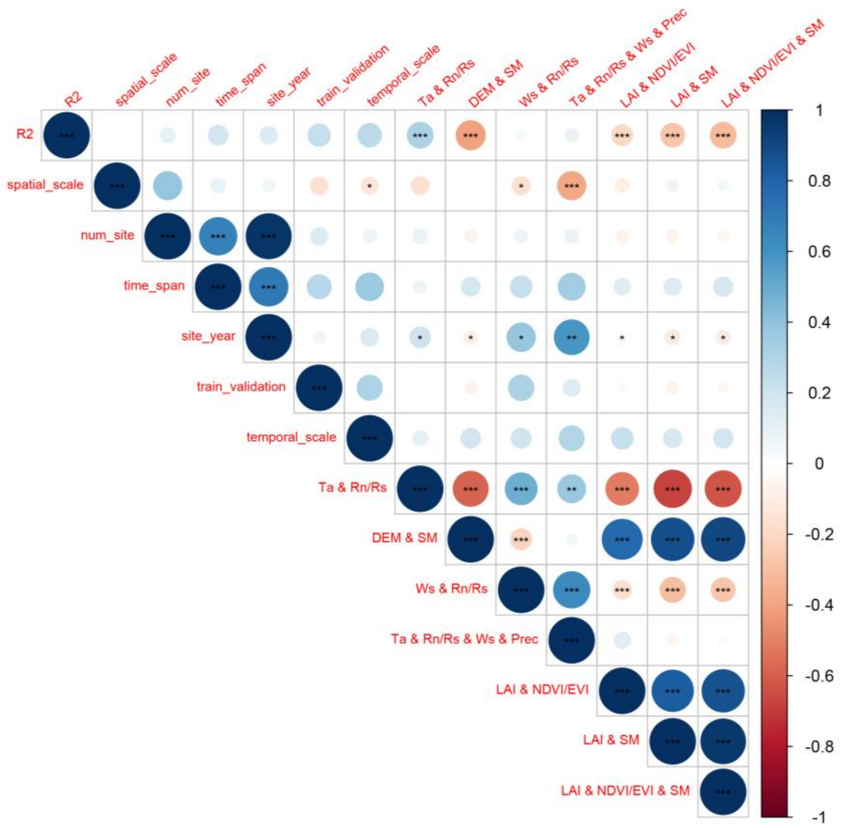


Figure 7. Evaluation of linear correlations between multiple features and the R-squared records with the statistical significance test. For the feature 'spatial scale', the 'local' scale was set to 1, the 'regional' scale was set to 2, and the 'global' scale was set to 3 in the analysis of linear correlation. For the use of various predictor combinations with '&', the value for 'together used' is set as 1 and other conditions are set as 0 (e.g., for the feature 'Ta & Rn/Rs & Ws & Prec', if Ta, Rn/Rs, Ws, and Prec were used together in the model, the value is set as 1). Significance: the p-value < 0.01 (***), 0.05 (**), and 0.1 (*).

4 Discussions

With the accumulation of in situ EC observations around the world~~, compared to remote sensing or process model-based approaches~~, the study of ET simulations based on data-driven approaches has received more attention from researchers in the last decade. Many studies have combined EC observations, various predictors, and machine learning algorithms to improve the prediction accuracy of site-scale water fluxes. To date, the results of these studies have not been comprehensively evaluated to provide clear guidance for feature selection in water flux prediction models. To better understand the approach and guide future research, we performed a meta-analysis of such studies. Machine learning-based water flux simulations and predictions still suffer from high uncertainty. By investigating the expected improvements that can be achieved by incorporating different features, we can avoid practices that may reduce model accuracy in future research.

4.1 Opportunities and challenges in the site-scale water flux simulation

In the above meta-analysis of the models, we found that water flux simulations based on EC observations can achieve high accuracy but also have high uncertainty through the modeling workflow. The R-squared of many water flux simulation models exceeds 0.8, possibly higher than some remote sensing-based and process-based models, and possibly higher than carbon flux simulations ~~in the same modeling framework. This suggests that in general, these currently used biophysical and meteorological variables are closely related to water fluxes.~~such as the net ecosystem exchange (Shi et al., 2022) in the same modeling framework.

Biophysical and meteorological variables are considered both important in ET simulations. This study found that models using a combination of meteorological variables had higher accuracy than models using only remotely sensed vegetation dynamic information. However, due to the high proportion of models with small temporal scales (e.g., half-hourly scale, hourly scale, and daily scale) in this study, this advantage of the combination of meteorological variables may be more suitable for small temporal scales. A possible explanation is that vegetation-related variables such as NDVI and LAI at the daily scale, 8-day scale, and 16-day scale have limited explanatory ability for hourly or daily-scale variability in ET. At a small temporal scale, the use of combinations of meteorological variables can capture moisture and energy conditions that control the rapid fluctuations of ET and thus has a dominant role in hourly or daily-scale ET prediction. This also corroborates the high accuracy of some physic-based ET estimation models (Rigden and Salvucci, 2015) that use only meteorological variables and not vegetation-related variables such NDVI (only an estimate of vegetation height derived from land cover maps is used to represent vegetation conditions (Rigden and Salvucci, 2015)).

There are differences in model accuracy among different PFTs. For example, in forest sites, limitations in data accuracy of factors were possible because some remote sensing-based predictors such as ~~FAPAR and LAI have limited accuracy when applied to forest types(Liu et al., 2018b).~~NDVI, FAPAR, and LAI have limited accuracy when applied to forest types (Liu et al., 2018b; Zeng et al., 2022). In addition, factors such as crown density, which may significantly affect the proportion of soil evaporation, transpiration, and evaporation of canopy interception, were not considered in these models, which may also lead to low model accuracy. This suggests that in water flux simulation, the driving mechanisms of water fluxes in different PFTs do affect the accuracy of machine learning models, and we need to consider more the actual and specific influencing factors in specific PFTs. More variables that can quantify the ratio of evaporation and transpiration should be considered for inclusion, which also appears to improve the mechanistic interpretability of such machine learning models. ~~Several studies~~A previous study (Zhao et al., 2019) ~~have~~has combined the physics-based approach (e.g., Penman-Monteith equation) and machine learning to build hybrid models to improve interpretability. We should make full use of empirical knowledge and experiences from process-based models to improve the accuracy and interpretability of the machine learning approach.

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~~The impact of differences in different satellite images on model accuracy and performance may be limited since most studies used windows of 2 km x 2 km or 3 km x 3km when extracting covariates based on satellite remote sensing(Walther et al., 2021) and the effects of differences in image resolution were smoothed out (i.e., the differences in values averaged over a 2 km window may not be significant at 30m and 500m resolutions). However, the coarse resolution of MODIS images may not be effective when the extraction window is smaller (e.g., 200 m) to reduce the inconsistency of the flux footprint extent and the extracted covariates from remote sensing images due to the non-homogeneity of the underlying conditions (Chu et al., 2021). Compared to the 16-daily temporal scale of Landsat data, the daily or 8-daily temporal scale of MODIS data may improve the accuracy slightly possibly because more temporal dynamic information is explained. The inclusion of some ancillary variables that do not have the temporal dimension (e.g., soil texture, topographic variables) may be of more limited use unless the model includes many flux sites for which the spatial variability of the ancillary variables is large enough and does affect water fluxes.~~

Among the ~~different~~ validation methods, random cross-validation has higher accuracy than spatial cross-validation and temporal cross-validation. However, spatial cross-validation and temporal cross-validation may be able to better help us recognize the robustness of the model when extrapolated (i.e., applied to new stations and new years). The lower accuracy in the temporal cross-validation approach implies that we need to focus on interannual hydrological and meteorological variability in the water flux simulations. In cropland sites, we may also need to pay more attention to the effects of interannual variability in anthropogenic cropping patterns. If some extreme weather years are not included, the robustness of the model when extrapolated to other years may be challenged, especially in the context of the various extreme weather events of recent years. This can also inform the siting of future flux stations. Regions where climate extremes may occur and biogeographic types not covered by existing flux observation networks should be given more attention to achieve global-scale, accurate and robust machine learning-based spatio-temporal prediction of water fluxes.

4.2 Uncertainties and limitations of this meta-analysis

4.2.1 The ~~potential uncertainties and limitations of the results of this meta-analysis are as follows:~~

~~The~~**limited number of available literature and model records** ~~that can be collected:~~

~~a)~~ Despite many articles and model records collected through our efforts to perform this meta-analysis, there still appears to be a long way to go to finally and completely understand the various mechanisms involved in water flux simulation with machine learning. Some of the insights provided by this study can be not robust (due to the limited sample size available when the goal is to assess the effects of multiple features), but this does not negate the fact that this study does obtain some meaningful findings. Therefore, researchers should treat the results of this study with caution, as they were obtained only statistically. Overall, it is still positive to conduct a meta-analysis of such studies, considering their rapid growth in the number and lack of guiding directions.

4.2.2 Publication bias and weighting

~~b)~~ Publication bias and weighting: Due to the relatively limited number of articles that could be included in the meta-analysis, this study did not focus much on publication bias. Meta-analytic studies in other fields

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typically measure the quality of journals and the public availability of research data (Borenstein et al., 2011; Field and Gillett, 2010) to determine the weighting ~~in~~of the literature in a comprehensive assessment. However, most of the articles did not publicly provide flux observations or share developed models. Meta-analysis studies in other fields typically measure the impact of included studies based on sample size and variance of experimental results (Adams et al., 1997; Don et al., 2011; Liu et al., 2018a). In this study, due to the lack of a convincing manner to determine weights among articles, we assigned the same weight to the results for all the literature.

4.2.3 Uncertainties in the information of the extracted features~~: First, as most studies used far more water flux observation records than~~

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At the ~~number of covariates in their regression models, we did not adjust~~information extraction level, the ~~R-squared in this study to an adjusted R-squared. Secondly,~~following issues may also introduce uncertainties:

a) Uncertainties caused by data quality control (e.g. gap-filling (Hui et al., 2004)) ~~and differences in the eddy covariance observation instruments used to observe water fluxes, etc., are difficult to assess effectively. Thirdly, the~~are difficult to assess effectively. Gap-filling is a commonly used technique to fill in low-quality data in flux observations (Chen et al., 2012; Hui et al., 2004). However, the impact of this practice on machine learning-based ET prediction models is unclear, due to the difficulty of directly assessing how this technique is performed in various studies by this meta-analysis. Typically, models with small time scales (e.g., hourly scale, daily scale) can exclude low-quality observations and use only high-quality data. However, for models with large time scales (e.g., monthly scales), gap-filling (e.g., based on meteorological data) may be unavoidable. This may lead to decrease in training data purity and introduce uncertainty in the subsequent prediction model development.

b) Systematic uncertainties caused by the energy balance closure (EBC) issue in eddy-covariance flux measurements are also difficult to assess by this meta-analysis. EBC is a common problem (Eshonkulov et al., 2019) in eddy-covariance flux observations. For that reason, the latent heat flux measured potentially underestimates ET. Some prediction models corrected EBC (e.g., using Bowen ratio preserving (Mauder et al., 2013, 2018) and energy balance residuals (Charuchittipan et al., 2014; Mauder et al., 2018)) in the processing of training data, but some did not. How this will affect the accuracy of the prediction model is not clear due to multiple factors that need to be evaluated that influence EBC (Foken, 2008), including measurement errors of the energy balance components, incorrect sensor configurations, influences of heterogeneous canopy height, unconsidered energy storage terms in the soil-plant-atmosphere system, inadequate time averaging intervals, and long-wave eddies (Jacobs et al., 2008; Foken, 2008; Eshonkulov et al., 2019). To reduce this uncertainty, more attention to flux site characteristics (Eshonkulov et al., 2019) related to PFT, topography, flux footprint area, etc., to select the appropriate correction method is necessary for future studies.

c) As most studies used far more water flux observation records than the number of covariates in their regression models, we did not adjust the R-squared in this study to an adjusted R-squared.

d) The various specific ways in which the parameters of the model are optimized are not differentiated. They are broadly categorized into different families or kinds of algorithms, which may also introduce uncertainty into the assessment.~~ Fourth, the~~

~~c)~~e) The assessment of some features is not detailed due to the limitations of the available model records. For example, the classification of PFT could be more detailed. ‘Forest’ could be further classified as broadleaf forest, coniferous forest, etc. while ‘cropland’ could be further classified as rainfed and irrigated cropland based on differences in their response mechanisms of water fluxes to environmental factors.

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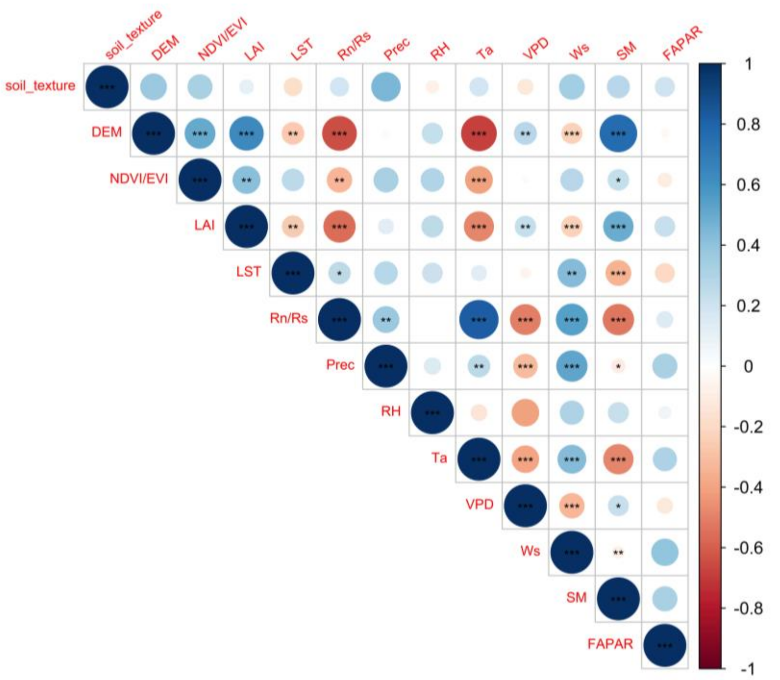
~~d) Independence between features: There is dependence between some of the features being evaluated, which may affect the assessment of the impact of single features on the accuracy of the model. We found that the use of NDVI/EVI, LAI, VPD, and SM was significantly negatively correlated with the use of Rn/Rs and Ta (Fig. 7) when unused was set to 0 and used was set to 1. It means that many of the models that used Rn/Rs and Ta did not use NDVI/EVI, LAI, VPD, and SM, and the models that used NDVI/EVI, LAI, VPD, and SM also happened to not use Rn/Rs and Ta. It can indirectly explain the fact that the accuracy of the models with NDVI/EVI, LAI, VPD, and SM is even lower than that of the models without NDVI/EVI, LAI, VPD, and SM in the above analysis (Fig. 5) because of the disturbance from the use of Rn/Rs and Ta.~~



~~Fig. 7. Correlation matrix between the use of various predictors (not used is set as 0 and used is set as 1) which may introduce uncertainty in the assessment of the impact of an individual predictor on model performance. Significance: the p-value < 0.01 (***), 0.05 (**), and 0.1 (*).~~

5 Conclusion

We performed a meta-analysis of the site-scale water flux simulations combining in situ flux observations, meteorological, biophysical, and ancillary predictors, and machine learning. The main conclusions are as follows:

~~a)~~1. SVM (average R-squared = 0.82) and RF (average R-squared = 0.81) outperformed over evaluated algorithms with sufficient sample size in both cross-study and intra-study (with the same training dataset) comparisons.

~~b)~~2. The average accuracy of the model applied to arid regions is higher than in other climate ~~classes~~types.

~~c)~~3. The average accuracy of the model was slightly lower for forest sites (average R-squared = 0.76) than for cropland and grassland sites (average R-squared = 0.8 and 0.79), but higher than for shrub sites (average R-squared = 0.67).

~~d)~~4. Among various predictor variables, the use of Rn/Rs, Prec, Ta, and FAPAR improved the model accuracy. The combination of Ta and Rn/Rs is very effective especially in the forest type, while in the grassland type the combination of Ws and Rn/Rs is also effective.

~~e)~~5. Among the different validation methods, random cross-validation shows higher model accuracy than spatial cross-validation and temporal cross-validation.

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Author Contributions

~~Haiyang Shi: Conceptualization, Methodology, Data, Writing. Geping Luo: Conceptualization, Supervision, Revision. Olaf Hellwich: Methodology. Alishir Kurban: Supervision. Tim Van De Voorde: Supervision. Philippe De Maeyer: Supervision, Revision. Xiaofei Ma, Xiuliang Yuan, Yuangang Wang, Wenqiang Zhang, Mingjuan Xie, Chen Zhang, Yu Zhang: Data.~~

HS and GL were responsible for the conceptualization, methodology, formal analysis, investigation, visualization, and writing. OH contributed to the investigation. XM, XY, YW, WZ, MX, CZ and YZ processed the data. AK, TVDV and PDM provided supervision.

Competing interests

The authors declare that they have no conflict of interest.

Code availability

The codes that were used for all analyses are available from the first author (shihaiyang16@mails.ucas.ac.cn) upon request.

Data availability

The data used in this study can be accessed by contacting the first author (shihaiyang16@mails.ucas.ac.cn) ~~based on reasonable~~upon request.

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