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Selecting essential factors for predicting reference crop evapotranspiration through tree-based machine learning and Bayesian optimisation

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Abstract: Reference crop evapotranspiration (ET_0) is a basic component of the hydrological cycle, and its estimation is critical for agricultural water resource management and scheduling. In this study, three tree-based machine learning algorithms (random forest [RF], gradient boosting decision tree [GBDT], and extreme gradient boosting [XGBoost]) were adopted to determine the essential factors for ET_0 prediction. The tree-based models were optimised using the Bayesian optimisation (BO) algorithm, and they were compared with three standalone models in terms of daily ET_0 and monthly mean ET_0 estimation in North China, with different input combinations of essential variables. The results indicated that solar radiation (R_s) and air temperature (T_s), including the maximum, minimum, and average temperature, in daily ET_0 were the key parameters affecting model prediction accuracy. R_s was the most influential factor in the monthly average ET_0 model, followed by T_s . Both relative humidity (RH) and wind speed at 2 m (U_2) had little impact on ET_0 prediction at different scales, although their importance differed. Compared with the GBDT and RF models, the XGBoost model exhibited the highest performance for daily ET_0 and monthly mean ET_0 estimation. The hybrid tree-based models with the BO algorithm outperformed the standalone tree-based models. Overall, compared with other inputs, the model with three inputs (R_s , T_s , and RH/U_2) had the highest accuracy. The BO-XGBoost model exhibited superior performance in terms of the global performance index (GPI) for daily ET_0 and monthly mean ET_0

prediction and it is recommended as a more accurate model predicting daily ET_O and monthly mean ET_O in North China or areas with a similar climate.

Keywords: Reference crop evapotranspiration; Essential factors; Tree-based algorithms; Machine learning; Bayesian optimization

1. Introduction

Reference crop evapotranspiration (ET_O) is the core indicator for crop water resource management and water-saving irrigation planning (Hai et al., 2018; Yu et al., 2020; Zhao et al., 2020). The accurate estimation of ET_O is critical for the efficient utilisation of water resources and the implementation of precision agriculture.

Many methods have been applied for measuring ET_O , with the experimental measurement method being the most scientific. However, this method is challenging due to its complex experimental operations and expensive materials. Therefore, various low-cost mathematical methods for predicting ET_O have been proposed, such as the United Nations Food and Agriculture Organization Penman–Monteith (FAO-56 PM; Pereira et al., 2015; Zhao et al., 2021), Hargreaves (HG), Jensen–Haise, and Imark–Allen methods. Among them, the FAO-56 PM method has been widely used given its wide applicability and high accuracy. However, this method requires many meteorological input factors, T_s , R_s , RH , and U_2 (Wang et al., 2020); these comprehensive meteorological data are often not easily obtainable, which limits the practical applications of this method (Abdullah et al., 2015; Fan et al., 2018; Wang et al., 2020; Wu et al., 2019). Few-factor ET_O estimation methods, such as the Hargreaves–Samani and Priestley–Taylor models, have also been widely employed, but they cannot respond to complicated processes or be effectively optimised (Fan et al., 2018; Saeid et al., 2017; Wu et al., 2019). Therefore, the construction of a few-factor ET_O model is a key research objective. Evapotranspiration is a nonlinear regression process involving various

50 meteorological factors. Machine learning has obvious advantages for managing complex nonlinear
51 data and has the potential to estimate ET_0 (Feng et al., 2016; Yin et al., 2017). Wu and Fan (2019)
52 estimated ET_0 using several machine learning algorithms (i.e., support vector machine [SVM],
53 M5Tree, and extreme gradient boosting [XGBoost]) and models to achieve reliable results when
54 only temperature data was used as input. Abdullah et al. (2015) compared the prediction
55 capabilities of the elaboration likelihood model (ELM) model with that of the FAO-56 PM and
56 FFBP model and determined the ELM algorithm to have higher accuracy, faster speed, and greater
57 generalisability; thus, this model is suitable for use in places with similar climatic conditions to
58 Iraq. Feng et al. (2016) examined the accuracies of the temperature-based ELM and generalised
59 regression network neural network model (GRNN) models for estimating ET_0 in the Sichuan Basin
60 in China, and they described that these two machine learning models outperformed the
61 temperature-based HG model. Thus, researchers have demonstrated that machine learning models
62 can estimate ET_0 with high accuracy. Among the algorithms used for regression, tree-based
63 ensemble models, such as the M5Tree and RF models, have been widely applied given their
64 convenient processes and accurate results (Muhammed et al., 2017). Armin et al. (2014) used the
65 M5Tree model and artificial neural network, with the surface temperature of five weather stations
66 in south-eastern Iran as input data, and they reported the model's estimation as remarkable. Feng
67 et al. (2017) documented that the RF model outperformed the empirical Iqbal model in predicting
68 daily diffuse R_s in North China. Shiri (2018) combined the RF model with the wavelet algorithm;
69 when calculating ET_0 in southern Iran, the performance of the RF model was markedly higher than
70 that of traditional and empirical models. Zhang et al. (2020) compared the precision of the CatBoost
71 model with that of the GRNN model tested and trained using meteorological data from 1996 to
72 2015, including daily maximum temperature ($T_{\max}$), daily minimum temperature ($T_{\min}$), wind speed

at 2 m (U_2), RH, and net radiation (R_n); they concluded that CatBoost was more effective than the GRNN model. Wu et al. (2019) proposed various machine learning models to predict ET_O using only local or cross-site temperature data and observed that tree models had higher estimation accuracy than other machine learning models. Overall, tree-based machine learning algorithms have exhibited strong performance in ET_O model construction research.

However, machine learning models have a high computation time and require numerous input parameters for data training. Most of the input parameters of the tree-based models in the aforementioned studies were selected based on experience and without a theoretical basis. The selection of effective essential principal factors for ET_O model construction is crucial. Some scholars have adopted principal component analysis to simplify multiple variables into a few essential variables. Through path analysis, Liu et al. (2017) identified essential meteorological variables for neural network estimation models in Wuhan and Guangzhou to simplify parameters, which allowed for a broad model application range and value. Muhammad et al. (2017) verified that the dimensionality of data was reduced through principal component analysis. The accuracy of ET_O prediction reached 83% without lacking key parameters, which is more accurate than ET_O prediction using other models. Although the use of the principal component analysis method to extract the main input factors is both scientific and feasible, the aforementioned study had certain regional limitations. Moreover, this method is mainly used for linear problems and is not ideal for solving nonlinear problems. Machine learning can solve nonlinear problems more effectively, and the use of the tree model to select the main factors is thus more suitable. To improve the prediction accuracy of SVR in the modelling of daily ET_O , Babak and Saeid (2020) applied RF and principal component preprocessing to recognise the optimal inputs, concluding that the RF process generated more accurate results than other approaches.

96 To construct a high-accuracy ET_O model, we selected 12 stations in North China for ET_O
97 prediction using a tree-based model. The study objectives were as follows: (1) use RF, GBDT, and
98 XGBoost to select essential factors for daily ET_O and monthly mean ET_O prediction; (2) compare
99 the RF, GBDT, XGBoost, and hybrid tree-based (Bayesian optimisation [BO]-RF, BO-GBDT, and
100 BO-XGBoost) models in terms of predicting daily ET_O and monthly mean ET_O with the essential
101 factors; and (3) evaluate all tree-based models and identify the model with the most effective
102 performance in North China on different time scales.

103 **2. Materials and methods**

104 *2.1 Study area*

Fig. 1. Geographic distribution of the meteorological stations in North China.

The area of North China (110°–120°E and 32° – 42°N) includes Beijing, Tianjin, Hebei, Shanxi, and the Inner Mongolia Autonomous Region (Fig. 1). The climate of the study area is dominated by a temperate monsoon and subtropical monsoon climate. The environmental changes are distinct across the four seasons: winter is cold and dry, summer is hot and rainy, and spring is dry with less precipitation and strong evaporation. The amount of precipitation is insufficient, and precipitation is unevenly distributed throughout the year, with most rainfall occurring in summer. The annual precipitation is 500–1000 mm, with 600–700 mm in the lower Yellow River plain and

500–600 mm in the area around Beijing and Tianjin.

The meteorological data from 1960 to 2019 were obtained from China Meteorological Data Network (<http://data.cma.cn>). Table 1 is a detailed description of weather stations. The data were divided into the training set (80%) and test set (20%); to reduce mistakes and improve the generalisability of the model, a 10-fold cross-validation method was adopted (Fig. 2).

Table 1

Geographical locations and mean daily values of the meteorological data of the 12 weather stations in this study.

Station ID	Station name	Latitude (°N)	Longitude (°E)	Elevation (m)	$T_{\max}$ (°C)	$T_{\min}$ (°C)	RH (%)	U_2 (m s ⁻¹)	n (h d ⁻¹)	ET_o (mm d ⁻¹)
50527	Hailaer	49.22	119.75	139.3	5.3	-6.5	0.6	2.3	7.2	2.0
50548	Xiaoergou	49.12	123.43	139.3	8.3	-7.3	0.7	1.2	7.2	1.8
53391	Huade	41.90	114.00	286.1	9.5	-2.6	0.6	3.0	8.2	2.6
53487	Datong	40.06	113.20	1039.3	14.1	0.7	0.5	2.0	7.4	2.8
53513	Linhe	40.44	107.22	778.3	14.9	2.0	0.5	1.7	8.7	2.9
53772	Taiyuan	37.47	112.33	76.8	17.3	4.3	0.6	1.5	6.9	2.8
53798	Xingtai	37.04	114.30	376.0	19.7	9.1	0.6	1.4	6.4	2.9
53868	Linfen	36.04	111.30	995.9	19.3	7.5	0.6	1.2	5.9	2.7
54012	WestUjimqin	44.35	117.36	842.8	8.7	-4.6	0.6	2.7	7.8	2.4
54311	Weichang	41.58	117.46	2.1	12.3	-0.6	0.6	1.4	7.5	2.3
54449	Qinhuangdao	39.51	119.31	54.0	15.7	6.4	0.6	1.8	7.1	2.6
54511	Beijing	39.48	116.28	54.0	18.2	7.5	0.6	1.8	7.2	3.0

Note: average air temperature (T_{mean}), maximum air temperature (T_{max}), minimum air temperature (T_{min}), average relative humidity (RH), sunshine hours (n), and average wind speed at 2 m (U_2).

2.2 FAO-56 PM equation

In this study, we used the FAO-56 PM equation ((Mirza and Kyung, 2018), 2018) as the target output of the machine learning model in model training and testing, as proposed by Allen et al. (1998).

$$ET_0 = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T+273} U_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34U_2)} \quad (1)$$

where Δ is the slope of the saturation vapour pressure temperature curve ($\text{kPa } ^\circ\text{C}^{-1}$); R_n is the net solar radiation at the crop surface ($\text{MJ m}^{-2}\text{d}^{-1}$); G is the soil heat flux density ($\text{MJ m}^{-2}\text{d}^{-1}$); γ is the psychrometric constant ($\text{kPa}^\circ\text{C}^{-1}$); U_2 is the mean daily wind speed at the height of 2 m (m s^{-1}), which is calculated from the logarithmic wind speed profile at 10 m; e_s is the saturation vapour pressure (kPa); e_a is the actual vapour pressure (kPa); and T is the mean air temperature at the height of 2 m ($^\circ\text{C}$).

The angstrom formula was applied to calculate R_s .

$$R_s = (a_s + b_s \frac{n}{N}) R_a \quad (2)$$

where R_s is the solar radiation ($\text{MJ m}^{-2}\text{day}^{-1}$); n is the actual sunshine duration (h); N is the maximum possible sunshine duration (h); n / N is the relative sunshine duration; and R_a is the zenith radiation ($\text{MJ m}^{-2}\text{day}^{-1}$), which also acts as the regression constant. The part of zenith radiation that reaches the ground in cloudy weather is ($n = 0$), with $a_s + b_s$ representing the part of zenith radiation reaching the ground on a sunny day ($n = N$); in this paper, the parameter values indicated in the FAO-56 PM are $a_s = 0.25$, $b_s = 0.50$.

2.3 Data processing

Prior to the input processing of the importance ranking of the input data features, the data must be normalised. In this study, min–max normalisation was used.

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)} \quad (3)$$

where x and x' represent the original and normalised data, respectively.

2.4 Tree-based algorithms

2.4.1 RF

RF is an algorithm that was introduced by Breiman (2001). To ensure the effectiveness of the decision tree, multiple bootstrap sampling is employed to obtain numerous random samples, with hundreds of decision trees forming a random forest. The nodes of each decision tree are randomly generated, and the partition variables of each node are created through the random selection of a few variables.

Because RF can assess the relationship between covariates and dependent variables and calculate the relative importance of covariates, this model can be used for feature ordering and selection. In this study, the impurity reduction method was applied to calculate feature importance. The importance of a feature can be measured based on the extent of the reduction in impurity in all trees in the forest that this feature induces. The score for each feature is calculated after training, and the results are standardised, resulting in a summed importance of all features that is equal to 1. The following Gini index calculation method was also applied:

$$\text{Gini}(p) = \sum_{k=1}^K p_k(1 - p_k) \quad (4)$$

where k represents the k categories, and p_k represents the sample weight of category k .

The importance on node m is the change in the Gini index before and after the branch of node m , which can be expressed as

$$\text{VIM}_{jm}^{(\text{Gini})} = \text{GI}_m - \text{GI}_l - \text{GI}_r \quad (5)$$

where GI_l and GI_r represent the Gini index of the two new nodes after branching, respectively.

The feature is X_j , and the node that appears in decision tree i is in the set M . The importance of X_j in the i -th tree is as follows:

$$\text{VIM}_{ij}^{(\text{Gini})} = \sum_{m \in M} \text{VIM}_{jm}^{(\text{Gini})} \quad (6)$$

For RF, assuming that n represents the total number of trees, the feature importance is given by

$$VIM_j^{(Gini)} = \sum_{i=1}^n VIM_{ij}^{(Gini)} \quad (7)$$

For regression problems, the final result of RF calculation is the average of all tree results. The regression process is described as follows:

First, k training samples $(\theta_1, \theta_2, \dots, \theta_k)$ are randomly generated from the total training sample using the bootstrap sampling method, corresponding to K decision trees that can be constructed.

At each node of the decision tree, m features are randomly selected from M features as the splitting feature set of the current nodes. When one node is selected from m features for splitting the feature set according to the principle of minimum node purity, each decision tree is grown to the largest extent possible, with no pruning.

For new data, the predictive value of a single decision tree can be obtained by averaging the observations of the leaf node $1(x, \theta)$. If an observation value X_i is a leaf node $1(x, \theta)$ and not 0, the weight $\omega_i(x, \theta)$ is set as follows:

$$\omega_i(x\theta) = \frac{1_{\{x_i \in R_l(x, \theta)\}}}{\#\{j: x_j \in R_l(x, \theta)\}} \quad (8)$$

where the sum of weights equals 1.

The prediction of a single decision tree obtained through the weighted average of the observations of dependent variables is defined as follows:

$$\mu(x) = \sum_{i=1}^n \omega_i(x\theta) Y_i \quad (9)$$

where Y_i ($i = 1, 2, \dots, n$) is the observation of the dependent variables.

According to the weight of the decision tree $\omega_i(x\theta_t)$ ($t = 1, 2, \dots, k$), the weight of each observation is computed as in Eq. (4).

$$\omega_i(x) = \frac{1}{k} \sum_{i=1}^k \omega_i(x\Theta_t)Y_i \quad (10)$$

Thus, the final predicted value of RFR is

$$\mu(x) = \sum_{i=1}^n \omega_i(x)Y_i \quad (11)$$

2.4.2 GBDT

GBDT is a representative algorithm in the boosting series that is widely used in classification and regression (Fan et al., 2018). We used the squared error to represent the loss function, through which each regression tree learns the conclusions and residuals of all previous trees, which are fit to obtain the current residual regression tree. The residual is equal to the real value subtracted by the predicted value, and the lifting tree is the accumulation of the regression tree generated through the whole iterative process.

Taking the hypothetical training set sample $T = (x, y_1), (x, y_2), \dots, (x, y_m)$, the maximum number of iterations is T , loss function is L , and output is a strong learner $f(x)$. The regression algorithm process is as follows:

The weak learner is initialised, and the mean value of C can be set to the mean value of sample y .

$$f_0(x) = \underset{c}{\operatorname{argmin}} \sum_{i=1}^m L(y_i, c) \quad (12)$$

The number of iterations $t = 1, 2, 3, \dots, T$ for sample $i = 1, 2, 3, \dots, m$ is used to calculate the negative gradient as follows:

$$r_{ti} = - \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right]_{f(x)=f_{t-1}(x)} \quad (13)$$

$(x_i, r_{ti}) i = 1, 2, 3, \dots, m$ is used to fit a classification and regression tree (CART) to obtain the t -th regression tree. The corresponding leaf node area is $R_{tj}, j = 1, 2, 3, \dots, J$, where J is the number of leaf nodes of regression tree t .

216 For the leaf area $j = 1, 2, 3, \dots, J$, the best-fit value is calculated as follows:

$$217 \quad c_{tj} = \underbrace{\operatorname{argmin}_c}_{\substack{\text{argmin} \\ c}} \sum_{x_i \in R_{tj}} L(y_i, f_{t-1}(x_i) + c) \quad (14)$$

218 The strong learner $f(x)$ is updated,

$$219 \quad f_t(x) = f_{t-1}(x) + \sum_{j=1}^J c_{tj} I(x \in R_{tj}) \quad (15)$$

220 and the $f(x)$ expression is obtained as follows:

$$221 \quad f(x) = f_T(x) = f_0(x) + \sum_{t=1}^T \sum_{j=1}^J c_{tj} I(x \in R_{tj}) \quad (16)$$

222 2.4.3 XGBoost

223 XGBoost is a regression-oriented algorithm proposed by Chen and Guestrin (2016). The
 224 algorithm uses much fewer resources than other systems to expand billions of examples. In the
 225 training process, parallel computing is automatically realised. Compared with other factors, the
 226 relative importance of input factors is determined, and the built-in cross-validation model assists
 227 in preventing model overfitting, which can provide a more reliable explanation for the results.
 228 XGBoost integrates multiple regression tree models to form a strong classifier, thereby increasing
 229 the training speed, parallel processing, and generalisability. Furthermore, with more data, the
 230 parallel efficiency is higher.

231 XGBoost can be regarded as an additive model composed of K CARTs.

$$232 \quad \hat{y}_i = \sum_{k=1}^K f_k(x_i) \quad f_k \in F \quad (17)$$

233 where K is the number of trees; F is all possible CARTs; and f_k is a specific CART.

234 In the return process, with the parameters $\theta = \{f_1, f_2, \dots, f_k\}$, the objective function of XGBoost
 235 becomes

$$236 \quad O(\theta) = \sum_{i=1}^N l(y_i, \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (18)$$

The first part of the formula presents the loss function, and the second part is the regular term, which is obtained through the addition of the regularisation terms of the K trees.

Through vector mapping for each tree, the decision tree is improved, and the regularisation term of XGBoost is obtained as follows:

$$\Omega(f_t) = \gamma T + \frac{1}{2} \lambda \sum_{j=1}^T \omega_j^2 \quad (19)$$

where γ and λ are the penalty coefficients of the model; T is the number of leaf nodes; and ω is the fraction of leaves.

The optimisation objective function is gradually approached step by step. At step t , an optimised CART is added on the basis of $t - 1$, and the objective function becomes

$$O(t) = \sum_{i=1}^N l(y_i, \hat{y}^{(t)}) + \sum_{i=1}^t \Omega(f_i) = \sum_{i=1}^N l(y_i, \hat{y}^{(t-1)} + f_t(x_i)) + \Omega(f_t) \quad (20)$$

Second-order Taylor expansion of this formula is then calculated to obtain

$$O(t) = \sum_{i=1}^N [l(y_i, \hat{y}^{(t-1)}) + g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i)] + \Omega(f_t) \quad (21)$$

$$g_i = \frac{\partial(l(y_i, \hat{y}^{(t-1)}))}{\partial \hat{y}^{(t-1)}} \quad (22)$$

$$h_i = \frac{\partial^2(l(y_i, \hat{y}^{(t-1)}))}{\partial \hat{y}^{(t-1)^2}} \quad (23)$$

where g_i and h_i are the first and second derivatives of the loss function, respectively.

2.5 BO algorithm

When the calculation is complex and the number of iterations is high, BO can be applied. BO is usually used for hyperparameter determination. For an optimised objective function, the posterior distribution of the objective function can be updated through the continual addition of sample points until the posterior distribution largely fits the real distribution. BO has two core

257 processes, namely prior function (PF) and acquisition function (AC). PF mainly uses Gaussian
 258 process regression, whereas AC includes expected improvement, the probability of improvement,
 259 the upper confidence bound of these methods, and the balance of exploration and exploitation. To
 260 achieve exploration, a point far away from the known point is selected as the reference point for
 261 the next iteration (to explore the unknown area), with the point distribution computed as evenly as
 262 possible. For exploitation, a point close to the known point is selected as the reference point for the
 263 next iteration (to exploit the points around the known point), with points distributed in a dense area,
 264 facilitating achievement of the local maximum.

265 If a set of hyperparameter combinations $X = x_1, x_2, \dots, x_n, x_n$ represents the value of a
 266 certain hyperparameter, BO assumes a functional relationship between the hyperparameters and
 267 the loss function that requires optimisation. For example, take the function $f: X \rightarrow \mathbb{R}$, $X \subset$
 268 $\mathbb{R}^n, n \in N$. In each iteration, $f(x_t), x_t \in X (t = 1, 2, \dots, T)$ is obtained according to the AC.
 269 Then, $y_t = f(x_t) + \varepsilon$ is obtained, with ε obeying the zero mean Gaussian distribution $\varepsilon \sim$
 270 $\mathcal{N}(0, \sigma^2)$; σ denotes the variance. The new observation data (x_t, y_t) are added to the original
 271 observation data, and the next iteration is then executed. Through the learning of the objective
 272 function, BO uses the information of the previous sampling point to identify the parameters that
 273 would improve and move the result toward the global optimum. The algorithm tests the most
 274 probable point in the posterior distribution. Fig. 2 depicts the entire analytical process of the
 275 optimisation model for estimating ET_O .

Fig. 2. Flowchart of the reference crop evapotranspiration prediction model used in this study

2.5 Model prediction evaluation

The coefficient of determination (R^2), root mean squared error (RMSE), mean absolute error (MAE), Nash–Sutcliffe efficiency coefficient (NSE), and GPI were used to evaluate the performance of the models (Feng et al., 2015; Shiri et al., 2015).

$$R^2 = \frac{\left[\sum_{i=1}^n Si - \bar{s} (Oi - \bar{O}) \right]^2}{\sum_{i=1}^n Si - \bar{s}^2 \sum_{i=1}^n (Oi - \bar{O})^2} \quad (22)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (Si - Oi)^2} \quad (23)$$

$$NSE = 1 - \frac{\sum_{i=1}^n (Si - Oi)^2}{\sum_{i=1}^n (Oi - \bar{O})^2} \quad (24)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |Si - Oi| \quad (25)$$

$$GPI = \alpha_j \sum_{i=1}^4 \left(T_j - \bar{T}_j \right) \quad (26)$$

where X_i and Y_i are the simulated and measured values, respectively; n is the number of measured

values; and $\bar{x}$ and $\bar{y}$ are the means of the simulated and measured values, respectively. T_j is the normalised value of RMSE, MAE, R^2 , and NSE, and $\bar{T}_j$ is the median of the corresponding parameter; when T_j is RMSE and MAE, α_j is -1 or 1 otherwise. The closer R^2 is to 1 , the more accurate is the prediction ability of the model, and the smaller the value of MAE and RMSE, the smaller the simulation error. The closer NSE is to 1 , the higher the model quality and credibility. The higher the GPI, the more effective the overall simulation effect of the model.

3. Results

3.1 Factor importance analysis based on tree-based algorithms

Three tree-based algorithms, namely RF, GBDT, and XGBoost, were applied to determine the essential meteorological factors for daily ET_O and monthly mean ET_O prediction. Importance weights between 0 and 1 were assigned to T_{max} , T_{min} , T_{mean} , RH, U_2 , and R_s in these three methods, with the importance being used to determine the most effective meteorological factors on different time scales. Fig. 3 and Fig. 4 present the results of the factor importance analysis based on the tree-based algorithms according to the heat map. Overall, the algorithms exhibited varying performance in the daily ET_O and monthly mean ET_O factor importance analysis, but the importance tended to be consistent on the same time scale.

For the daily ET_O factor importance analysis (Fig. 3 and Table 2) in five selected sites in Inner Mongolia (50527, 50548, 53391, 53513, and 54012), T_s was the most important influencing factor, ranging from 0.717 to 0.795 , 0.675 to 0.867 , and 0.721 to 0.794 for RF, GBDT, and XGBoost, respectively, followed by R_s , ranging from 0.115 to 0.216 , 0.091 to 0.250 , and 0.116 to 0.218 , respectively. Among the other sites selected in North China, R_s was the most influential factor, ranging from 0.700 to 0.759 , 0.499 to 0.680 , and 0.699 to 0.758 for RF, GBDT, and XGBoost,

respectively, followed by T_s , ranging from 0.115 to 0.228, 0.245 to 0.421, and 0.152 to 0.229, respectively. RH and U_2 consistently ranked third and fourth in importance at all sites.

In the factor importance analysis of the monthly mean ET_O , R_s had the most importance at all study sites, ranging from 0.638 to 0.970, 0.855 to 0.967, and 0.567 to 0.857 for RF, GBDT, and XGBoost, respectively (Fig. 4 and Table 2). After R_s , T_s exhibited the most importance, ranging from 0.021 to 0.035, 0.022 to 0.136, and 0.128 to 0.410 for RF, GBDT, and XGBoost, respectively, followed by RH and U_2 .

Most of the importance analysis results of the three models on the daily and monthly scales were the same. Because the contribution of R_s and T_s differed considerably in different regions, we used R_s and T_s as the basic input combination, with both input at the same time. Finally, RH and U_2 were introduced. (Table 3).

Fig. 3. Heat map of the factor importance analysis of daily ET_O .

Fig. 4. Heat map of the factor importance analysis of monthly mean ET_O .

Table 2

Factor importance analysis of daily ET_O and monthly mean ET_O .

Daily ET_O							Monthly mean ET_O					
Station	T_{mean}	T_{max}	T_{min}	U_2	RH	R_s	T_{mean}	T_{max}	T_{min}	U_2	RH	R_s
RF							RF					
50527	0.279	0.512	0.004	0.035	0.036	0.135	0.046	0.297	0.007	0.003	0.009	0.638
50548	0.724	0.009	0.005	0.027	0.019	0.216	0.118	0.083	0.012	0.003	0.005	0.778
53391	0.032	0.698	0.004	0.048	0.047	0.171	0.007	0.063	0.009	0.004	0.010	0.907
53487	0.069	0.136	0.004	0.049	0.042	0.700	0.011	0.022	0.007	0.005	0.008	0.947
53513	0.518	0.196	0.003	0.062	0.025	0.196	0.012	0.021	0.005	0.006	0.005	0.952
53772	0.047	0.122	0.004	0.054	0.029	0.744	0.005	0.013	0.003	0.004	0.005	0.970
53798	0.037	0.148	0.006	0.055	0.036	0.717	0.017	0.039	0.012	0.021	0.010	0.902
53868	0.032	0.192	0.004	0.043	0.028	0.702	0.008	0.033	0.003	0.003	0.005	0.948
54012	0.710	0.067	0.004	0.056	0.048	0.115	0.021	0.095	0.004	0.006	0.008	0.867
54311	0.174	0.023	0.007	0.031	0.016	0.749	0.026	0.019	0.015	0.003	0.005	0.932
54449	0.120	0.052	0.025	0.037	0.042	0.724	0.034	0.051	0.035	0.008	0.007	0.864
54511	0.055	0.075	0.022	0.059	0.031	0.759	0.014	0.023	0.011	0.004	0.010	0.938
GBDT							GBDT					
50548	0.578	0.281	0.008	0.015	0.027	0.091	0.016	0.091	0.009	0.004	0.011	0.870
53399	0.719	0.018	0.011	0.015	0.024	0.213	0.019	0.094	0.023	0.004	0.005	0.855
53446	0.081	0.567	0.028	0.027	0.052	0.246	0.003	0.103	0.014	0.005	0.011	0.863
53463	0.167	0.239	0.015	0.031	0.049	0.499	0.003	0.022	0.015	0.004	0.010	0.946
53513	0.479	0.212	0.008	0.029	0.022	0.250	0.011	0.027	0.002	0.006	0.008	0.946
53772	0.112	0.176	0.018	0.045	0.044	0.605	0.006	0.015	0.001	0.004	0.006	0.967
53798	0.114	0.235	0.019	0.037	0.039	0.555	0.018	0.042	0.005	0.025	0.008	0.901
53959	0.084	0.244	0.019	0.035	0.030	0.587	0.005	0.036	0.003	0.004	0.005	0.948
54012	0.527	0.274	0.006	0.022	0.044	0.127	0.001	0.112	0.001	0.005	0.008	0.872
54135	0.345	0.056	0.018	0.022	0.020	0.539	0.015	0.005	0.031	0.004	0.004	0.942
54311	0.191	0.091	0.046	0.035	0.026	0.610	0.014	0.047	0.031	0.011	0.008	0.890
54449	0.122	0.078	0.044	0.040	0.035	0.680	0.003	0.022	0.029	0.006	0.011	0.929
XGBoost							XGBoost					
50548	0.015	0.776	0.003	0.035	0.034	0.137	0.020	0.378	0.012	0.005	0.018	0.567
53399	0.721	0.011	0.002	0.030	0.017	0.218	0.185	0.135	0.005	0.007	0.004	0.664
53446	0.012	0.712	0.003	0.048	0.045	0.180	0.024	0.192	0.010	0.006	0.012	0.757
53463	0.069	0.139	0.003	0.050	0.040	0.699	0.085	0.127	0.010	0.010	0.009	0.759
53513	0.657	0.061	0.003	0.063	0.024	0.192	0.023	0.106	0.002	0.007	0.005	0.857

53772	0.049	0.127	0.003	0.051	0.033	0.738	0.086	0.038	0.004	0.009	0.008	0.855
53798	0.040	0.148	0.004	0.057	0.035	0.717	0.160	0.049	0.020	0.020	0.013	0.738
53959	0.036	0.190	0.002	0.043	0.028	0.700	0.051	0.170	0.006	0.007	0.007	0.759
54012	0.719	0.057	0.003	0.053	0.052	0.116	0.105	0.138	0.002	0.007	0.016	0.732
54135	0.178	0.021	0.006	0.032	0.017	0.747	0.090	0.047	0.003	0.006	0.003	0.851
54311	0.133	0.052	0.016	0.039	0.040	0.721	0.112	0.037	0.138	0.011	0.004	0.698
54449	0.034	0.096	0.023	0.060	0.030	0.758	0.065	0.061	0.015	0.009	0.011	0.839

Table 3

Input combinations of the meteorological factors for various models.

Models						Input combinations
RF	GBDT	XGBoost	BO-RF	BO-GBDT	BO-XGBoost	
Daily ET ₀ predicting						
RF1	GBDT1	XGBoost1	BO-RF1	BO-GBDT1	BO-XGBoost1	R _s
RF2	GBDT2	XGBoost2	BO-RF2	BO-GBDT2	BO-XGBoost2	T _s
RF3	GBDT3	XGBoost3	BO-RF3	BO-GBDT3	BO-XGBoost3	R _s , T _s
RF4	GBDT4	XGBoost4	BO-RF4	BO-GBDT4	BO-XGBoost4	R _s , T _s RH
RF5	GBDT5	XGBoost5	BO-RF5	BO-GBDT5	BO-XGBoost5	R _s , T _s U ₂
Monthly mean ET ₀ predicting						
RF6	GBDT6	XGBoost6	BO-RF6	BO-GBDT6	BO-XGBoost6	R _s
RF7	GBDT7	XGBoost7	BO-RF7	BO-GBDT7	BO-XGBoost7	T _s
RF8	GBDT8	XGBoost8	BO-RF8	BO-GBDT8	BO-XGBoost8	R _s , T _s
RF9	GBDT9	XGBoost9	BO-RF9	BO-GBDT9	BO-XGBoost9	R _s , T _s RH
RF10	GBDT10	XGBoost10	BO-RF10	BO-GBDT10	BO-XGBoost10	R _s , T _s U ₂

3.2. Comparison of daily ETo and monthly mean ETo models with different input combinations

The performance of the tree-based models (RF, GBDT, and XGBoost) and the hybrid tree-based models (BO-RF, BO-GBDT, and BO-XGBoost) under different input combinations in both the training and testing phase in terms of RMSE, R², MAE, and NSE is summarised in Table 4. Boxplots of the performance of the tree-based models and hybrid tree-based models on the daily and monthly mean scale under different input combinations in the testing phase are illustrated in Fig. 5 and Fig. 6. The same letter denotes no significant difference between the models, as determined using Fisher's least significant difference at a 0.05 significance level.

As presented in Fig. 5, for daily ET_O estimation, no significant difference was observed between the R_s and T_s input ($p > 0.05$), indicating the similar overall accuracy of these two factors. When the two factors were input, the difference was obvious compared with single-factor input ($p < 0.05$). Three-factor input considerably improved the accuracy of most models; however, the RF model did not exhibit a marked improvement compared with the two-factor input condition. Compared with the accuracy of the single-factor model, the three-input RF model showed significantly improved performance ($p < 0.05$). No significant difference was noted among the three-factor combinations (with RH or U_2) in terms of the model accuracy indicators ($p > 0.05$), which was consistent with the main factor analysis result. As illustrated in Fig. 5, for monthly average ET_O estimation, a significant correlation was found between the single-factor and double-factor input, exhibiting the same trend as that of daily ET_O . When two factors were input, the difference was obvious compared with single-factor input ($p < 0.05$). Three-factor input considerably improved the accuracy of most models, but the RF model did not show marked improvement compared with the two-factor input model. However, the three-input RF model showed significant improvement in terms of accuracy compared with the single-factor model ($p < 0.05$). No significant difference was noted among the three-factor combinations (with RH or U_2) in terms of the model accuracy indicators ($p > 0.05$). Compared with single-factor input, the accuracy of the three-factor input model considerably improved, but the accuracy of the two-factor input model did not exhibit significant improvement ($p > 0.05$).

As detailed in Table 4, under the different input combinations, the XGBoost models outperformed the other models in the training phase, with RMSE, R^2 , MAE, and NSE ranging from 0.316 to 0.821 mm d^{-1} , 0.796 to 0.969, 0.220 to 0.623 mm d^{-1} , and 0.796 to 0.969, respectively, and from 0.335 to 0.836 mm d^{-1} , 0.789 to 0.966, 0.232 to 0.633 mm d^{-1} , and 0.789 to 0.966,

respectively, in the testing phase; this was followed by the performance of the GBDT and RF models. In addition to the significance difference between the standalone and hybrid models, significant differences were observed in R^2 , RMSE, MAE, and NSE under different input combinations, indicating that the hybrid BO algorithm significantly improved the tree-based algorithms. No significant difference was noted among the three hybrid models, with all hybrid models exhibiting high accuracy compared with the standalone tree-based models. Overall, the BO-XGBoost model had highest accuracy among the other tree-based models in the training phase RMSE, R^2 , MAE, and NSE ranging from 0.263 to 0.737 mm d⁻¹, 0.834 to 0.979, 0.182 to 0.555 mm d⁻¹, and 0.834 to 0.979, respectively, and from 0.317 to 0.811 mm d⁻¹, 0.801 to 0.969, 0.214 to 0.606 mm d⁻¹, and 0.801 to 0.969, respectively, in the testing phase; this was followed by the performance of the BO-GBDT and BO-RF models.

The BO-XGBoost model had the highest accuracy along with the other tree-based models, and the XGBoost models outperformed the GBDT models, followed by the RF models. The accuracy of the model increased with the increased number of input parameters, which is consistent with the main factor results.

Table 4

R^2 , RMSE, MAE, and NSE values of ET_O prediction during the training and testing phases.

Input	Training				Testing			
	RMSE (mm d ⁻¹)	R^2	MAE (mm d ⁻¹)	NSE	RMSE (mm d ⁻¹)	R^2	MAE (mm d ⁻¹)	NSE
R_s								
RF1	0.832±0.119	0.790±0.034	0.633±0.076	0.790±0.034	0.841±0.129	0.786±0.039	0.638±0.081	0.786±0.039
GBDT1	0.822±0.119	0.795±0.034	0.624±0.077	0.795±0.034	0.837±0.131	0.789±0.040	0.634±0.083	0.789±0.040
XGBoost1	0.821±0.119	0.796±0.034	0.623±0.077	0.796±0.034	0.836±0.131	0.789±0.040	0.633±0.083	0.789±0.040
BO-RF1	0.824±0.120	0.794±0.036	0.627±0.077	0.794±0.036	0.840±0.129	0.787±0.039	0.637±0.081	0.787±0.039
BO-GBDT1	0.746±0.149	0.830±0.047	0.558±0.103	0.830±0.047	0.815±0.139	0.799±0.045	0.607±0.096	0.799±0.045
BO-XGBoost1	0.737±0.139	0.834±0.043	0.555±0.096	0.834±0.043	0.811±0.141	0.801±0.046	0.606±0.096	0.801±0.046
T_s								
RF2	0.852±0.096	0.775±0.053	0.634±0.091	0.775±0.053	0.865±0.093	0.769±0.054	0.643±0.089	0.769±0.054
GBDT2	0.792±0.092	0.806±0.044	0.584±0.084	0.806±0.044	0.806±0.088	0.800±0.042	0.595±0.081	0.800±0.042
XGBoost2	0.772±0.090	0.815±0.044	0.568±0.083	0.815±0.044	0.791±0.084	0.808±0.041	0.582±0.080	0.808±0.041
BO-RF2	0.812±0.086	0.796±0.046	0.600±0.082	0.796±0.046	0.825±0.085	0.791±0.046	0.610±0.080	0.791±0.046
BO-GBDT2	0.713±0.094	0.842±0.044	0.527±0.085	0.842±0.044	0.778±0.086	0.815±0.039	0.572±0.080	0.815±0.039

BO-XGBoost2	0.709±0.081	0.846±0.024	0.522±0.067	0.846±0.024	0.745±0.072	0.831±0.023	0.547±0.065	0.831±0.023
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R _s , T _s								
RF3	0.645±0.081	0.874±0.018	0.467±0.060	0.874±0.018	0.659±0.085	0.869±0.019	0.476±0.060	0.869±0.019
GBDT3	0.514±0.086	0.919±0.017	0.356±0.065	0.919±0.017	0.539±0.091	0.912±0.019	0.370±0.068	0.912±0.019
XGBoost3	0.515±0.086	0.919±0.017	0.356±0.066	0.919±0.017	0.539±0.091	0.912±0.019	0.370±0.068	0.912±0.019
BO-RF3	0.576±0.083	0.899±0.017	0.406±0.062	0.899±0.017	0.592±0.086	0.894±0.018	0.417±0.062	0.894±0.018
BO-GBDT3	0.492±0.096	0.926±0.02	0.340±0.071	0.926±0.02	0.530±0.093	0.915±0.019	0.363±0.069	0.915±0.019
BO-XGBoost3	0.473±0.094	0.931±0.02	0.327±0.068	0.931±0.02	0.529±0.093	0.915±0.019	0.360±0.069	0.915±0.019
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R _s , T _s , RH								
RF4	0.642±0.077	0.875±0.016	0.464±0.058	0.875±0.016	0.655±0.081	0.870±0.017	0.473±0.057	0.870±0.017
GBDT4	0.359±0.068	0.961±0.010	0.247±0.049	0.961±0.010	0.382±0.071	0.956±0.010	0.260±0.050	0.956±0.010
XGBoost4	0.358±0.068	0.961±0.010	0.247±0.049	0.961±0.010	0.381±0.072	0.956±0.011	0.259±0.050	0.956±0.011
BO-RF4	0.543±0.065	0.910±0.012	0.387±0.052	0.910±0.012	0.560±0.067	0.905±0.012	0.398±0.051	0.905±0.012
BO-GBDT4	0.322±0.075	0.968±0.010	0.220±0.052	0.968±0.01	0.367±0.073	0.959±0.010	0.244±0.051	0.959±0.010
BO-XGBoost4	0.305±0.070	0.971±0.010	0.208±0.050	0.971±0.01	0.366±0.070	0.959±0.010	0.241±0.049	0.959±0.010
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R _s , T _s , U ₂								
RF5	0.638±0.079	0.876±0.016	0.461±0.057	0.876±0.016	0.651±0.083	0.872±0.017	0.469±0.057	0.872±0.017
GBDT5	0.315±0.049	0.969±0.008	0.219±0.035	0.969±0.008	0.335±0.053	0.966±0.009	0.231±0.038	0.966±0.009
XGBoost5	0.316±0.049	0.969±0.008	0.22±0.036	0.969±0.008	0.335±0.054	0.966±0.009	0.232±0.039	0.966±0.009
BO-RF5	0.527±0.061	0.916±0.012	0.376±0.048	0.916±0.012	0.541±0.065	0.911±0.013	0.386±0.049	0.911±0.013
BO-GBDT5	0.265±0.065	0.978±0.010	0.183±0.047	0.978±0.010	0.319±0.058	0.969±0.009	0.215±0.042	0.969±0.009
BO-XGBoost5	0.263±0.056	0.979±0.007	0.182±0.038	0.979±0.007	0.317±0.055	0.969±0.009	0.214±0.040	0.969±0.009
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R _s								
RF6	0.71±0.062	0.802±0.019	0.597±0.055	0.802±0.019	0.690±0.056	0.807±0.025	0.568±0.051	0.807±0.025
GBDT6	0.135±0.027	0.992±0.003	0.107±0.021	0.992±0.003	0.391±0.059	0.934±0.019	0.286±0.039	0.934±0.019
XGBoost6	0.308±0.055	0.961±0.014	0.236±0.041	0.961±0.014	0.370±0.060	0.943±0.018	0.278±0.042	0.943±0.018
BO-RF6	0.394±0.034	0.938±0.011	0.308±0.026	0.938±0.011	0.402±0.043	0.934±0.015	0.310±0.034	0.934±0.015
BO-GBDT6	0.294±0.119	0.96±0.024	0.224±0.090	0.960±0.024	0.392±0.071	0.937±0.020	0.293±0.048	0.937±0.020
BO-XGBoost6	0.349±0.064	0.95±0.017	0.270±0.049	0.950±0.017	0.366±0.064	0.944±0.019	0.277±0.045	0.944±0.019
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T _s								
RF7	0.772±0.065	0.764±0.03	0.631±0.058	0.764±0.03	0.747±0.078	0.774±0.032	0.599±0.068	0.774±0.032
GBDT7	0.065±0.015	0.998±0.001	0.049±0.012	0.998±0.001	0.504±0.090	0.889±0.038	0.344±0.054	0.889±0.038
XGBoost7	0.318±0.049	0.959±0.013	0.239±0.039	0.959±0.013	0.447±0.063	0.918±0.021	0.323±0.047	0.918±0.021
BO-RF7	0.571±0.057	0.87±0.025	0.449±0.056	0.870±0.025	0.580±0.071	0.863±0.027	0.454±0.067	0.863±0.027
BO-GBDT7	0.055±0.019	0.999±0.001	0.041±0.014	0.999±0.001	0.461±0.060	0.913±0.024	0.322±0.045	0.913±0.024
BO-XGBoost7	0.311±0.060	0.959±0.021	0.232±0.047	0.959±0.021	0.431±0.059	0.924±0.019	0.312±0.045	0.924±0.019
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R _s , T _s								
RF8	0.696±0.057	0.809±0.021	0.587±0.054	0.809±0.021	0.678±0.052	0.813±0.025	0.560±0.051	0.813±0.025
GBDT8	0.057±0.051	0.997±0.006	0.043±0.037	0.997±0.006	0.288±0.061	0.966±0.013	0.210±0.041	0.966±0.013
XGBoost8	0.147±0.039	0.991±0.004	0.108±0.027	0.991±0.004	0.219±0.045	0.980±0.007	0.158±0.026	0.980±0.007
BO-RF8	0.393±0.036	0.939±0.011	0.307±0.027	0.939±0.011	0.401±0.044	0.934±0.015	0.309±0.034	0.934±0.015
BO-GBDT8	0.072±0.087	0.996±0.006	0.053±0.064	0.996±0.006	0.249±0.048	0.974±0.009	0.179±0.032	0.974±0.009
BO-XGBoost8	0.152±0.051	0.990±0.006	0.112±0.038	0.990±0.006	0.213±0.045	0.981±0.007	0.155±0.029	0.981±0.007
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R _s , T _s , RH								
RF9	0.696±0.055	0.809±0.020	0.587±0.052	0.809±0.020	0.678±0.051	0.813±0.024	0.560±0.050	0.813±0.024
GBDT9	0.135±0.069	0.991±0.005	0.101±0.051	0.991±0.005	0.246±0.042	0.976±0.007	0.182±0.030	0.976±0.007
XGBoost9	0.107±0.024	0.995±0.002	0.079±0.018	0.995±0.002	0.177±0.039	0.987±0.006	0.128±0.025	0.987±0.006
BO-RF9	0.393±0.037	0.939±0.011	0.308±0.028	0.939±0.011	0.402±0.047	0.934±0.016	0.309±0.037	0.934±0.016
BO-GBDT9	0.054±0.059	0.998±0.003	0.041±0.044	0.998±0.003	0.200±0.047	0.983±0.007	0.146±0.036	0.983±0.007
BO-XGBoost9	0.102±0.029	0.996±0.003	0.074±0.022	0.996±0.003	0.167±0.037	0.989±0.004	0.122±0.026	0.989±0.004
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R _s , T _s , U ₂								
RF10	0.698±0.054	0.808±0.018	0.589±0.052	0.808±0.018	0.678±0.051	0.813±0.024	0.560±0.050	0.813±0.024
GBDT10	0.120±0.057	0.993±0.004	0.092±0.043	0.993±0.004	0.232±0.046	0.978±0.007	0.173±0.027	0.978±0.007
XGBoost10	0.101±0.018	0.996±0.001	0.075±0.014	0.996±0.001	0.168±0.030	0.989±0.003	0.124±0.021	0.989±0.003
BO-RF10	0.394±0.034	0.938±0.011	0.308±0.026	0.938±0.011	0.402±0.043	0.934±0.015	0.310±0.034	0.934±0.015
BO-GBDT10	0.060±0.066	0.997±0.004	0.046±0.051	0.997±0.004	0.193±0.041	0.985±0.005	0.141±0.029	0.985±0.005
BO-XGBoost10	0.082±0.025	0.997±0.002	0.061±0.018	0.997±0.002	0.158±0.032	0.990±0.003	0.117±0.022	0.990±0.003

Fig. 5. Statistical performance of daily ET_O prediction during testing under different input combinations.

Fig. 6. Statistical performance for monthly mean ET_0 prediction during testing under different input combinations.

3.3 GPI ranking of the daily ET_O and monthly mean ET_O models

Although RMSE, R^2 , MAE, and NSE were used, no single measure alone can be used to judge the performance of the tree-based models. Therefore, the GPI value was further calculated for all tree-based model at all stations under different input combinations (Table 5, Fig. 7, and Fig. 8). As listed in Table 5, the BO-XGBoost models, with GPI ranging from -1.954 to 1.938 , 0.402 to 1.837 , -0.459 to 1.982 , 0.436 to 1.966 , and 0.881 to 1.993 under the input factor(s) R_s ; T_s ; R_s and T_s ; R_s , T_s , and RH ; and R_s , T_s , and U_2 , respectively, exhibited the most effective performance at each station on the daily scale. The BO-XGBoost models also exhibited the highest GPI along with the other tree-based models on the monthly mean scale. Moreover, the hybrid tree-based models exhibited higher GPI compared with that of the standalone tree-based models at each station with different input combinations for the daily ET_O and monthly mean ET_O ; thus, the hybrid tree-based models outperformed the standalone tree-based models.

The GPI ranking comparison at each site in the study area is presented in Fig. 7 and Fig. 8. The smaller the circle radius, the larger the GPI value and the more satisfactory the model. In the comparison of daily ET_O GPI value rankings, the radius of the model with R_s input is larger than that with T_s input at the Inner Mongolia site, although the opposite is true for the other sites. This indicated that the T_s input of the Inner Mongolia site contributed more to the ET_O calculation than the R_s input, which is consistent with the results of the main factors. In the two-factor input combination, the radii of 50548 and 54311 were small, indicating that the accuracy of the model at these two sites was high; the importance of these two sites was closer to 1 than that of the other sites. When a third factor (RH or U_2) was introduced to the same site, the radius of the factor with greater importance was smaller than the factor with less importance, indicating that the model accuracy was less than the input combination with greater importance. Therefore, the importance

feature ranking was verified.

Table 5

Values of the global performance index and rankings of the tree-based models under different input combinations for daily ET_O and monthly mean ET_O during the testing phase.

Station ID	model	Daily scale					Monthly scale				
		R_s	T_s	R_s, T_s	R_s, T_s, RH	R_s, T_s, U_2	R_s	T_s	R_s, T_s	R_s, T_s, RH	R_s, T_s, U_2
50527	RF	-0.479	1.192	-0.543	-0.936	-0.933	-1.484	-0.731	-0.928	-1.043	-1.088
	GBDT	-0.467	1.610	0.876	1.364	1.423	0.819	-0.348	0.933	1.477	1.029
	XGBoost	-0.449	1.692	0.866	1.352	1.411	0.968	0.906	1.525	1.737	1.685
	BO-RF	-0.479	1.426	0.311	0.044	0.038	1.154	0.177	0.666	0.616	0.588
	BO-GBDT	-0.411	1.687	0.937	1.455	1.545	0.818	0.843	1.345	1.719	1.501
	BO-XGBoost	-0.383	1.776	1.004	1.512	1.575	0.939	1.026	1.586	1.763	1.741
50548	RF	1.104	1.041	0.414	-0.186	-0.197	-1.778	-0.230	-1.847	-1.710	-1.825
	BO-RF	1.147	1.542	1.843	1.863	1.833	1.115	0.980	1.749	1.620	1.639
	GBDT	1.148	1.745	1.834	1.859	1.860	1.239	1.651	1.914	1.923	1.892
	BO-GBDT	1.107	1.269	1.269	0.545	0.504	1.099	0.846	0.686	0.565	0.521
	XGBoost	1.404	1.742	1.977	2.000	2.000	1.002	1.366	1.810	1.915	1.948
	BO-XGBoost	1.495	1.837	1.982	1.966	1.993	1.211	1.688	2.000	2.000	1.973
53391	RF	-0.971	-0.255	-1.755	-1.737	-1.741	-1.289	-1.487	-1.470	-1.420	-1.488
	BO-RF	-0.958	-0.119	-0.417	0.715	0.723	1.278	0.736	1.212	1.143	1.427
	GBDT	-0.950	0.371	-0.415	0.712	0.718	1.507	1.140	1.562	1.691	1.624
	BO-GBDT	-0.969	0.092	-0.983	-0.750	-0.847	1.388	0.246	0.846	0.746	0.785
	XGBoost	-0.829	0.380	-0.382	0.810	0.739	1.495	1.079	1.452	1.422	1.463
	BO-XGBoost	-0.805	0.440	-0.366	0.856	0.881	1.514	1.068	1.601	1.755	1.691
53487	RF	0.067	-0.249	-1.445	-1.550	-1.588	-1.225	-1.736	-1.352	-1.376	-1.374
	BO-RF	0.100	-0.146	0.027	1.082	1.245	1.402	0.726	1.417	1.525	1.553
	GBDT	0.101	-0.145	0.021	1.100	1.258	1.710	1.144	1.558	1.830	1.776
	BO-GBDT	0.243	0.147	-0.533	-0.458	-0.422	1.225	0.071	0.807	0.701	0.647
	XGBoost	0.927	0.137	0.152	1.223	1.416	1.687	0.975	1.405	1.690	1.588
	BO-XGBoost	0.943	0.669	0.083	1.230	1.322	1.764	1.236	1.604	1.897	1.816
53513	RF	-0.322	0.168	-1.162	-1.418	-1.252	-1.130	-1.402	-1.287	-1.333	-1.339
	BO-RF	-0.288	0.567	-0.111	0.287	1.405	0.986	1.115	1.484	1.368	1.443
	GBDT	-0.282	0.692	-0.122	0.286	1.399	1.482	1.400	1.651	1.660	1.765
	BO-GBDT	-0.324	0.347	-0.556	-0.682	-0.150	1.232	0.206	0.716	0.689	0.662
	XGBoost	-0.138	0.674	-0.049	0.402	1.562	0.903	1.587	1.545	1.437	1.776
	BO-XGBoost	-0.038	0.709	-0.008	0.436	1.509	1.518	1.641	1.668	1.637	1.759
53772	RF	0.878	-0.288	-0.857	-1.184	-0.983	-0.932	-1.066	-1.195	-1.250	-1.172
	BO-RF	0.939	0.385	0.450	1.179	1.463	1.812	1.359	1.548	1.568	1.579
	GBDT	0.933	0.600	0.462	1.198	1.466	1.974	1.453	1.748	1.819	1.859
	BO-GBDT	0.879	0.094	-0.257	-0.395	0.007	1.420	0.167	0.896	0.816	0.801
	XGBoost	0.976	0.720	0.573	1.269	1.544	1.793	1.308	1.691	1.831	1.817
	BO-XGBoost	0.986	0.788	0.614	1.275	1.625	2.000	1.489	1.716	1.778	1.921
53798	RF	0.378	-0.746	-1.108	-1.383	-1.313	-1.639	-1.837	-1.656	-1.937	-1.755
	BO-RF	0.479	0.120	0.446	0.826	1.220	0.685	0.603	0.886	1.106	1.434

	GBDT	0.482	0.278	0.440	0.829	1.190	0.771	0.632	1.331	1.381	1.618
	BO-GBDT	0.384	-0.184	-0.173	-0.443	-0.248	0.516	-0.697	0.074	-0.063	0.036
	XGBoost	0.579	0.339	0.545	1.019	1.354	0.622	0.544	1.202	1.249	1.624
	BO-XGBoost	0.587	0.402	0.579	1.024	1.323	0.792	0.823	1.342	1.504	1.658
53868	RF	0.706	-0.032	-0.512	-0.937	-0.886	-1.046	-1.117	-1.218	-1.281	-1.338
	BO-RF	0.808	0.571	1.099	1.118	1.520	1.780	1.225	1.270	1.650	1.618
	GBDT	0.810	0.602	1.099	1.115	1.520	1.619	1.861	1.849	1.863	1.821
	BO-GBDT	0.710	0.533	0.327	-0.138	-0.001	0.943	0.587	0.547	0.445	0.401
	XGBoost	1.579	0.725	1.190	1.271	1.669	1.694	1.766	1.516	1.734	1.660
	BO-XGBoost	1.739	1.420	1.224	1.285	1.676	1.765	1.969	1.850	1.885	1.869
54012	RF	-2.000	0.423	-1.953	-1.939	-1.995	-0.996	-0.722	-1.190	-1.179	-1.138
	BO-RF	-1.984	0.816	-0.565	0.971	1.160	1.344	1.040	1.196	1.413	1.456
	GBDT	-1.989	0.909	-0.549	0.989	1.147	1.132	1.362	1.549	1.633	1.707
	BP-GBDT	-2.000	0.630	-1.150	-0.765	-0.745	1.041	0.609	0.568	0.494	0.496
	XGBoost	-1.942	0.891	-0.470	1.035	1.241	0.922	1.295	1.481	1.658	1.642
	BP-XGBoost	-1.954	0.966	-0.459	1.044	1.220	1.081	1.474	1.554	1.689	1.710
54311	RF	1.368	0.348	0.076	-0.439	-0.479	-0.919	-0.647	-1.107	-1.198	-1.162
	BO-RF	1.437	1.057	1.680	1.538	1.772	1.313	1.880	1.731	1.617	1.711
	GBDT	1.453	1.063	1.691	1.540	1.767	1.824	1.764	1.895	1.845	1.948
	BO-GBDT	1.370	0.718	0.881	0.222	0.261	1.451	0.891	0.926	0.846	0.823
	XGBoost	1.931	1.654	1.855	1.647	1.882	1.680	1.731	1.907	1.683	1.889
	BO-XGBoost	1.938	1.453	1.829	1.648	1.888	1.800	1.780	1.921	1.872	2.000
54449	RF	0.490	-1.363	-1.026	-1.296	-1.128	-0.821	-0.856	-0.914	-0.997	-1.010
	BO-RF	0.557	-0.538	0.618	1.523	1.058	1.051	0.188	1.185	1.482	1.558
	GBDT	0.565	-0.467	0.627	1.537	1.080	1.159	1.143	1.738	1.880	1.864
	BO-GBDT	0.489	-0.882	-0.049	-0.408	-0.324	1.269	0.726	0.681	0.703	0.657
	XGBoost	0.700	-0.433	0.623	1.676	1.170	1.024	0.840	1.361	1.772	1.720
	BO-XGBoost	0.734	0.593	0.619	1.653	1.178	1.141	1.221	1.758	1.929	1.877
54511	RF	0.856	-2.000	-1.472	-1.659	-1.376	-0.731	-1.199	-0.986	-1.068	-1.070
	BO-RF	0.899	-0.861	0.057	1.163	1.259	1.529	1.210	1.470	1.477	1.509
	GBDT	0.892	-0.649	0.060	1.169	1.255	1.577	1.023	1.722	1.824	1.745
	BO-GBDT	0.857	-1.338	-0.565	-0.644	-0.404	1.464	-0.273	0.896	0.838	0.839
	XGBoost	0.961	-0.347	0.204	1.279	1.342	1.572	1.271	1.654	1.771	1.495
	BO-XGBoost	0.942	0.747	0.263	1.280	1.410	1.641	1.292	1.752	1.847	1.777

Fig. 7. GPI value of the tree-based daily ET_0 prediction models during the testing phase.

Fig. 8. GPI rankings of the tree-based monthly mean ET_0 prediction models during the testing phase.

4. Discussion

4.1 Importance of meteorological data in daily ET_O and monthly mean ET_O estimation

The choice of dominant meteorological factors is critical to the prediction accuracy of machine learning ET_O prediction models. To analyse the importance of meteorological data to daily ET_O and monthly mean ET_O prediction, three tree-based algorithms (RF, GBDT, and XGBoost) were employed. The use of tree models to select essential factors for modelling ET_O can provide higher accuracy and stability with limited factors. Mohammadi et al. (2020) applied RF and four other methods for selecting the main factors of meteorological data to obtain accurate model prediction of daily ET_O . The results revealed that the SVM model under RF input factors exhibited the highest performance. In the factor importance analysis of daily ET_O and monthly mean ET_O , R_s was determined to be the primary driving factor of daily ET_O and monthly mean ET_O at almost all stations and at all stations, respectively. Additionally, Chen et al. (2019) reported that R_s was the key factor determining the accuracy of ET_O models in hilly areas. These results indicated that T_s and R_s were the main factors affecting ET_O . For daily ET_O , the performance of the importance analysis of the three algorithms was similar at each station. The primary influencing factor of meteorological stations in the Inner Mongolia Autonomous Region was T_s and in North China was R_s . Regarding the general characteristics of Inner Mongolia, T_s increases sharply in spring and during the short, hot summer and then suddenly decreases in autumn, followed by long, frosty, and severely cold winters. This may explain why T_s has a greater impact on daily ET_O estimation. In general, R_s and T_s accounted for more than 90% of the contribution to daily ET_O and monthly mean ET_O . The result of the feature importance calculation was clearly reflected in the prediction accuracy of the models.

4.2 Prediction accuracy of the tree-based machine learning models

To develop a more accurate model with broader application for predicting ET_O , we applied

RF, GBDT, and XGBoost to predict daily ETO and monthly mean ETO in North China based on the selected input combinations identified through factor importance analysis. On the monthly scale, the GBDT model outperformed the XGBoost model in the training phase with some input combinations but exhibited inferior performance to the XGBoost model in the testing phase. The GBDT model had an overfitting problem in which the new regression tree may have continuously fit the previous residuals, resulting in the residuals of the training set gradually approaching zero. Through a comparison of the tree-based models trained with different input combinations, we observed that the accuracy of the models predicting daily ETO and monthly mean ETO improved with the introduction of more factors. Furthermore, the XGBoost models outperformed the GBDT models in terms of R^2 , RMSE, MAE, NSE, and GPI, followed by the RF models. This result is consistent with that of Zhou et al. (2020), in which the XGBoost models outperformed GBDT and RF models. In this study, the daily ETO and monthly mean ETO models under different input combinations had high accuracy, demonstrating that the combination of essential factors obtained through factor importance analysis resulted in highly accurate modelling. The essential factor combination selected in the tree-based algorithm proved suitable and feasible for modelling daily ETO and monthly mean ETO.

4.3 Comprehensive evaluation of the hybrid BO models and standalone tree-based models

The BO algorithm was employed to identify the optimal parameter set for the relative model and to improve its accuracy (Alizamir et al., 2020; Min et al., 2021). In this study, BO was used to optimise RF, GBDT, and XGBoost, and effective results were obtained; the optimal parameter set successfully improved model accuracy and performance in the training and testing phases. Compared with the standalone tree-based models, the hybrid tree-based models (BO-RF, BO-GBDT, and BO-XGBoost) had higher performance in terms of RMSE, R^2 , MAE, NSE, and GPI,

with BO-XGBoost outperforming the other models (Fig. 7 and Fig. 8). Alibabaei et al. (2021) employed long short-term memory and bidirectional long short-term memory (BLSTM) to test ET_O in three locations in Portugal and applied BO to optimise the parameters of these machine learning models. The results demonstrated that BLSTM optimised with BO had the highest performance, which is consistent with the favourable optimisation effect reported in our study. In the training and testing phases, the BO algorithm exhibited satisfactory optimisation effects on the three tree-based ET_O models, with the three optimised models with three-input factor combinations exhibiting superior performance compared with the unoptimised models. However, when T_s and R_s were input, the hybrid BO models also performed well in daily ET_O estimation, with RMSE and MAE less than 0.592 mm d^{-1} and 0.417 mm d^{-1} , R^2 and NSE more than 0.894 and 0.894; for the monthly mean estimation, these were less than 0.402 mm d^{-1} and 0.310 mm d^{-1} , R^2 and NSE more than 0.934, and 0.934, respectively, with only R_s . This indicated that, in the absence of large amounts of data, only three factors can be used to predict monthly mean ET_O . This result clearly demonstrates that the selection of essential meteorological factors based on tree-based machine learning has strong rationality and reliability. Overall, the BO-XGBoost model with three factors is recommended for more accurate daily ET_O and monthly mean ET_O prediction in North China or in areas with a similar climate.

5. Conclusions

This study employed three tree-based machine learning algorithms (RF, XGBoost, and GBDT) to select essential factors for estimating daily ET_O and monthly mean ET_O , with the performance of these models and hybrid BO-optimised tree-based models evaluated at study sites in North China.

(1) The result of factor importance analysis indicated that R_s and T_s are the main factors affecting daily ET_O calculation, and R_s is the main factor affecting the calculation of the monthly average ET_O .

(2) Among the standalone tree-based models, the XGBoost model had the highest accuracy, followed by GBDT and RF. When inputting three factors (R_s , T_s , and U_2 or RH), the accuracy of the model predicting daily ET_O and monthly mean ET_O was the highest in terms of R^2 , RMSE, MAE, NSE, and GPI, followed by models that input one and two essential factors.

(3) The BO algorithm exhibited effective optimisation on the three tree-based models. The BO-XGBoost model had the highest accuracy, followed by the BO-GBDT and BO-RF models, in terms of R^2 , RMSE, MAE, NSE, and GPI. Under three-factor input (R_s , T_s , and U_2 or RH), this model exhibited the highest accuracy in modelling daily ET_O and monthly mean ET_O . Overall, BO-XGBoost with three-factor input is recommended as the prediction model for daily ET_O and monthly mean ET_O in North China.

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Data availability The datasets generated during and analysed during the current study are available from the corresponding author on reasonable request.

Code availability Not applicable.

Declarations

Ethics approval Not applicable.

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Conflict of interest The authors declare no competing interests.

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