



Boosting ensembles for estimation of discharge coefficient and through flow discharge in broad-crested gabion weirs

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Received: 29 September 2022 / Accepted: 30 November 2022 / Published online: 30 December 2022
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Abstract

Gabion weirs are environment-friendly structures widely used for irrigation and drainage network purposes. These structures' hydraulic performance is fundamentally different from solid weirs' due to their porosity and the existence of a through-flow discharge. This paper investigates the reliability and suitability of a number of Machine learning models for estimation of hydraulic performance of gabion weirs. Generally, three different Boosting ensemble models, including Gradient Boosting, XGBoost, and CatBoost, are compared to the well-known Random Forest and a Stacked Regression model, with respect to their accuracy in prediction of the discharge coefficient and through-flow discharge ratio of gabion weirs in free flow conditions. The Bayesian optimization approach is used to fine-tune model hyper-parameters automatically. Recursive feature elimination analysis is also performed to find optimum combination of features for each model. Results indicate that the CatBoost model has outperformed other models in terms of estimating the through flow discharge ratio (Q_{in}/Q_t) with $R^2 = 0.982$, while both XGBoost and CatBoost models have shown close performance in terms of estimating the discharge coefficient (C_d) with R^2 of CatBoost equal to 0.994 and R^2 of XGBoost equal to 0.992. Weakest results were also produced by Decision tree regressor with $R^2 = 0.821$ and 0.865 for estimation of C_d and Q_{in}/Q_t values.

Keywords Gabion weirs · Discharge coefficient · XGBOOST · CatBoost

Introduction

Gabion weirs are porous structures made of boulders with minimal construction cost and negative environmental effects (Yue et al. 2021, Zhang et al. 2019a,b). Generally, these structures benefit from higher stability, durability, and proper hydraulic performance (Zhang et al. 2019a,b, Fang et al. 2021, Liu et al. 2022). Besides, physical particles such

as sediments and chemical substances can pass through the porous body of these structures, which reduces sedimentation and increases flow aeration by increasing the downstream flow turbulence (Mohamed 2010; Fathi-moghaddam et al. 2018; Rahmanshahi and Bejestan 2020). The hydraulic performance of porous and solid broad-crested weirs has been studied experimentally (Azimi et al. 2013; Wüthrich and Chanson 2014; Zhang and Chanson 2016; Pirzad et al. 2021; Salmasi et al. 2021) and numerically (Jiang et al. 2018; Safarzadeh and Mohajeri 2018; Nourani et al. 2021, Yin et al. 2022a, b).

Even though solid and gabion weirs have similar geometrical shapes, the presence of the through flow highly affects their hydraulic performance (Shen et al. 2017, Chen et al. 2022). The relative diameter of filling particles is a dominant factor controlling their hydraulic performance by affecting the through flow discharge (Fathi-moghaddam et al. 2018). As a result, some researchers have concentrated on investigating how through and overflow interact under various submerged and free flow situations, and even some (Fathi-moghaddam et al. 2018; Shariq et al. 2020) have offered

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formulae to calculate through flow discharge. The effect of the broad-crested weir's geometrical shape is also extensively studied. Sargison and Percy (2009) state that Solid weirs' discharge coefficient decreases as the upstream slope increases. Madadi et al. (2014) experimentally investigated the effect of upstream slope on the discharge coefficient of broad crested weirs. They concluded that by increasing the slope of the upstream ramp, the separation zone dimensions increase, which reduces the discharge coefficient. According to (Fathimoghaddam et al. 2018) the material size significantly affects the weir behaviour. For larger filling particles, decreasing the slope of side ramps increases the upstream water head and subsequently lowers the discharge coefficient of gabion weirs, whereas, for smaller filling particles, a downstream slope enhances weir performance. The use of soft computing techniques in the field of hydraulic engineering has expanded to include a number of issues in recent years including estimation of sediment scour in streams (Pandey et al. 2020, 2022; Tao et al. 2021), hydraulic performance of solid weirs such as piano-key weirs (Olyaie et al. 2019; Zounemat-Kermani and Mahdavi-Meymand 2019), side-weirs (Dursun et al. 2012), labyrinth weirs (Norouzi et al. 2019; Wang et al. 2022), cylindrical weirs (Ismael et al. 2021), solid broad crested weirs (Hameed et al. 2021) and the hydraulic performance and energy dissipation of gabion weirs (Salmasi and Sattari 2017). However, two of the most utilized methods seem to be support vector machines (Azimi et al. 2019) and Feedforward neural networks (Khatibi et al. 2014). Utilizing an automated evolutionary hyperparameter optimization approach, Tao et al. (Tao et al. 2021) investigates the accuracy of proposed XGBoost-Ga method against some machine learning methods such as decision trees, support vector machines and linear regression and concludes that the proposed XGBoost-Ga method is the superior. Azimi et al. (Azimi et al. 2019) studied the ability of six different support vector machines to predict the discharge coefficient of side weirs. They suggested that the superior model is a function of the Froude number. Norouzi et al. (Norouzi et al. 2019) compared the performance of multilayer perceptron (MLP), support vector machines (SVM), and radial basis networks for estimation of the discharge coefficient of labyrinth weirs. They concluded that the *MLP* model outperforms other models.

Considering that the standalone models usually face the problem of overfitting, ensemble learning models have become widely used in different applications to reduce overfitting and increase the accuracy by combining diverse base learners (Yin et al. 2022a, b, Dai et al. 2022). Osman et al. (2021) compared the performance of artificial neural networks, SVMs and the XGBoost algorithm in terms of their accuracy for estimating the groundwater level in Malaysia. Their results indicated that for every considered combination of input models, the XGBoost outperforms other models. Jiajai et al. (Wu et al. 2022) evaluated the performance of ANNs and XGBoost in terms of their

accuracy in identifying leakages in water distribution networks. They concluded that the XGBoost outperforms the ANN by 5.54% in the estimation of leakage zone and by 2.7% in predicting the leakage level. Pham et al. (2021) evaluated the performance of different Boosting methods including Adaptive Boosting (AdaBost), Boosted Generalized Linear Models (BGLM), Extreme Gradient Boosting (XGB) ensemble models, and the Deep Boosting (DB) model in terms of their accuracy in estimating the flood hazard susceptibility of areas and suggested that DB model outperforms other model by 2%. More recent CatBoost ensemble model is also utilized in some studies including (Huang et al. 2019; Zhang et al. 2020; Guo et al. 2022) however it seems to be still unknown to the majority of hydraulic community. Zhang et al. (2020) evaluated the accuracy of CatBoost, Random forest, and the generalized regression neural network (GRNN) for estimation of daily evapotranspiration in arid regions and reported that CatBoost outperformed other models. On the other hand, Guo et al. (2022) compared the accuracy of CatBoost, XGBoost, and Neural networks with the genetic algorithm-based automated machine learning algorithm (Auto-ML) and reports that the Auto-ML model outperforms other model in terms of the accuracy in estimation of water logging depth and location in urban areas.

So far, different machine learning models have been utilized as surrogate models for estimation of the discharge coefficient of different solid weirs, yet only a few studies have focused on gabion weirs and no studies has considered the through flow of porous weirs due to the practical problems with their calculation and measurement resulted in the lack of a reliable dataset for such measurements. Besides, the application of ensemble models and specifically more recent and advanced models such as XGBoost and CatBoost models are also limited to few studies. Hence, this paper utilizes some base models including SVM, and Decision trees, along with some ensemble models such as Random Forest as a bagging ensemble, a Stacking ensemble model, and three different Boosting ensembles including Gradient Boosting Decision trees (GBDT), Extreme gradient Boosting model (XGB), and the more recent CatBoost model. Recursive feature elimination analysis is performed to find the optimal combination of features for each model. All models are then fine-tuned using the Bayesian hyper-parameter optimization method in order to improve their performance in estimation of the discharge coefficient and the through flow discharge of broad-crested gabion weirs.

Materials and method

Experimental data

In this study, experimental data of broad crested gabion weirs (Moradi and Fathi-Moghaddam 2014) and Salmasi et al. (2017) in free flow conditions are used to provide sufficient

Table 1 Geometrical and hydraulic characteristics of gabion weirs from experimental studies

Data source	$L_c(m)$	$P(m)$	$Q(l/s)$	$n(\%)$	$d_m(mm)$	upstream slope (α)	Downstream slope (β)
Salmasi et al. (2017)	0.15	0.15	–	39,41,45,50	5,10,15,30	90	90
Moradi and Fathi-moghaddam (2014)	0.15	0.15	3–30	43,44,46,47,50,51	7,11,14,17,22,31	30,45,60,90	30,45,60,90

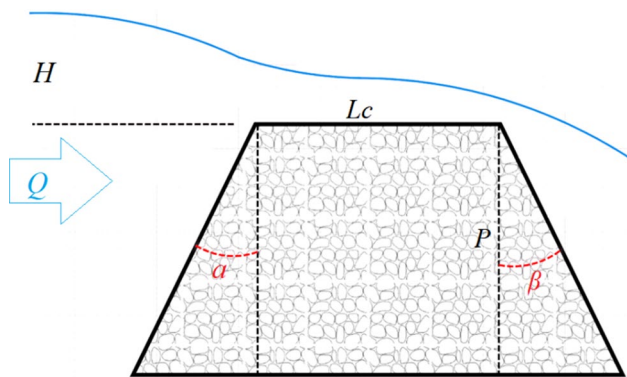


Fig. 1 Schematic view of the gabion weir parameters

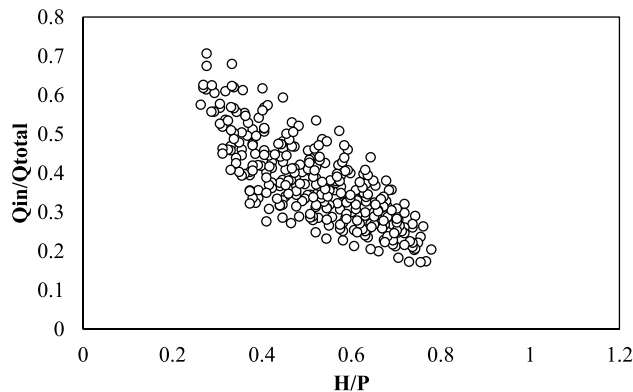


Fig. 3 Calculated through-flow discharge ratio

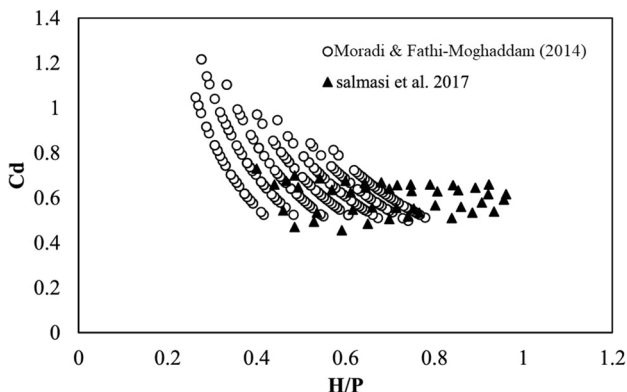


Fig. 2 Experimental C_d extracted from (Moradi and Fathi-Moghaddam 2014) and Salmasi et al. (2017)

data to train and test the models. The specifications of the experimental models are presented in Table 1 and Fig. 1. Experimental conditions include square weirs with 15×15 dimensions with different combinations of upstream and downstream slopes filled with particles with median diameters of 5–31 mm and a porosity of 39–51%. The discharge coefficients for the abovementioned models are presented in Fig. 2.

To calculate the discharge ratio through the porous body of gabion weirs, the multivariate regression equation suggested by Fathi-moghaddam et al. (2018) is utilized as follows:

$$Q_{in}/Q_{total} = 1.26 + 0.79\text{Log}(Re) - 4.82\left(\frac{H}{L_{crest}}\right)^{0.149} + 0.417\left(\frac{d_m}{p}\right) - 0.043 \tan(\alpha) + 0.013 \tan(\beta) \quad (1)$$

Calculated through flow ratio (Q_{in}/Q_t) of the abovementioned data using Eq. (1) is presented in Fig. 3.

Dimensional analysis

In free-flow conditions, discharge and discharge coefficient could be related as in Eq. (2). Hence, the effects of other hydraulic factors (i.e., weir geometry and fluid characteristics) must be taken into account in the calculation of C_d .

$$Q = \frac{2}{3} C_d B \sqrt{2g} H^{1.5} \quad (2)$$

where g is the gravitational acceleration, H is the total upstream head ($H = h + v^2/2g$), h is the head over the weir, and v is the approach velocity.

For a PE weir, the discharge coefficient, C_d , can be expressed by the following functional relationship:

$$f(C_d, h, L_c, P, Q, g, \sigma, \rho, \mu, d_{50}, \alpha, \beta, n) = 0 \quad (3)$$

in which f is a functional symbol, P is the weir height, ρ is water density, μ is water viscosity, and σ is surface tension.

Using the Π theorem of dimensional analysis (Barenblatt 1987) for the parameters in Eq. (2), the discharge coefficient for the free-flow condition can be expressed by the following dimensionless groups;

$$Cd = f\left(\frac{H}{P}, \frac{H}{Lc}, \frac{dm}{P}, Re, W, n, \tan(a), \tan(b)\right) \quad (4)$$

where Re is the Reynolds number; and W represents the Weber number.

Dataset preparation

In this paper, values of H lower than 4 cm over the weir are neglected to eliminate the effect of surface tension and hence the weber number. Values of H/Lc are also neglected as they are equivalent to H/P values. Consequently, the training dataset includes 6 features as input, including Re , H/P , d_m/P , n , $\tan(a)$, and $\tan(b)$, with all values Standardized using mean and standard deviation of values. Discharge coefficient data extracted from (Moradi and Fathi-Moghaddam 2014) includes 324 values for trapezoidal weirs, and those from Salmasi et al. (2017) include 44 data for rectangular weirs without upstream and downstream slopes. Hence, the whole dataset used to train and evaluate models includes 368 data points, of which 70% are used as training and 30% are used to evaluate the model performance. Correlation coefficients between different input and output features are presented in Fig. 4. It is clear that H/P values are highly correlated with the C_d and Q_{in} values. In addition, d_m/P , porosity (n), and upstream slope show a moderate correlation with the Q_{in} values.

Single and ensemble learning algorithms

Support vector machines (SVM)

SVMs (Cortes and Vapnik 1995) are a type of supervised machine learning algorithms with both applications in classification and regression which guarantees obtaining a global optimum solution. The core idea behind SVM is

that it assigns training samples to spatial coordinates in order to maximize the distance between the two categories. Then, depending on which side of the gap they fall, new samples are projected into that same area and predicted to belong to a category. Real-world issues are often more complicated, necessitating more accurate hypotheses than those offered by existing linear learning machines, which also have certain computing drawbacks. Thus, using different kernels (Aizerman and Control 1964) available such as Radial Basis Function (Azimi et al. 2019) and polynomial kernels would be useful in examining correlations among real-world situations in order to create a specific model. Support vector regression (SVR) is a supervised-learning technique that trains using a loss function that penalizes both high and low misestimates equally. Vapnik's ϵ -insensitive approach ignores absolute values of errors above and below the estimate that are fewer than a predefined threshold by constructing a flexible tube with a small radius symmetrically around the estimated function. In this fashion, although points outside the tube are penalized, points within the tube that are above or below the function are not. One of the main advantages of SVR is that its computational cost is independent of the size of the input space. Additionally, it has a significant generalization ability and decent prediction accuracy (Awad and Khanna 2015). This research evaluates RBF and polynomial Kernels in terms of their accuracy for predicting discharge coefficient and through flow discharge.

Decision Trees (DT)

A class of supervised learning techniques known as decision trees (Breiman et al. 1983) are a good example of a universal function approximator, despite the difficulty of achieving this universality in their fundamental structure. Classification and regression are both possible applications for them. A Decision Tree is a collection of branches that are linked by decision nodes and finish in leaf nodes (DT). The decision node of the tree includes several alternative leaf nodes that reflect the model output, with each branch representing an algorithmic option. As a label or a continuous value, this may be used in classification and regression. Decision nodes make up a large portion of the DT's structure. Using the smallest possible tree to minimize overfitting is a fundamental aim for machine learning models when it comes to correctly representing the relationships between input and output. An ensemble DT model (EDT) is often employed, in which a number of trees are utilized to generate a final model at once (i.e., bootstrap aggregation or bagging) or sequentially (i.e., boost) (Jain et al. 2020).

	dm/P	n	H/P	$\tan(a)$	$\tan(b)$	Cd	Q_{in}
dm/P	1.00	-0.52	-0.17	0.02	0.01	0.51	0.55
n	-0.52	1.00	0.01	0.12	0.12	-0.26	-0.53
H/P	-0.17	0.01	1.00	-0.13	-0.12	-0.65	-0.78
$\tan(a)$	0.02	0.12	-0.13	1.00	0.04	-0.10	-0.45
$\tan(b)$	0.01	0.12	-0.12	0.04	1.00	-0.19	-0.09
Cd	0.51	-0.26	-0.65	-0.10	-0.19	1.00	0.92
Q_{in}	0.55	-0.53	-0.78	-0.45	-0.09	0.92	1.00

Fig. 4 Correlation Matrix for Different features in the Dataset

Random forest regression (RFR)

An RFR method is a regression technique based on machine learning. Using bagging and random subspace as a foundation, RFR is a stable foundation upon which to develop. Hence, a number of learner trees are generated, which are then merged to get an overall prediction. To train the learning trees, original training data are used to generate bootstrap samples. Each bootstrap sample (Db) is created by randomly picking n instances from the original training data (D), which comprises N instances. It is possible to replace the bootstrap samples with fresh instances. Db is about two-thirds the size of D and contains no duplicate instances. Using the vector of input data, x, k distinct regression trees are constructed for each bootstrap sample. Low bias and high variance are characteristics of regression trees. Random forest predictions are generated by averaging the predictions of K regression trees, $h_k(x)$ (N. et al. 2021) as follows:

$$RFR_{\text{prediction}} = \frac{1}{k} \sum_{k=1}^k h_k(x) \tag{5}$$

Stacked regression

Stacking regressions first presented by (Breiman 1996) is a technique for combining many predictors linearly to enhance prediction accuracy. The algorithm mainly consists of 2 steps, including (1) specifying a list of base learners and training each on the dataset and (2) using the predictions of the base learners as input to train the value of the meta-learner and predict new values with the meta-learner. This study's defined structure of the stacked regression includes support vector machines with polynomial and RBF kernel along with Ridge regression as level-1 models and the Decision Tree Regressor as the Meta model, as depicted in Fig. 5.

Gradient boosting

Gradient Boosted Decision Trees (GBDT) (Friedman 2001) a supervised learning technique first introduced by Jerome H. Friedman starts with a set of $\{x_i, y_i\}$ values where x_i represent the input values and y_i are corresponding target values. The Gradient Boosting technique then involves iteratively creating a set of functions of $F^0, F^1, \dots, F^t, \dots, F^m$ which are then used to form the corresponding loss function $L(y_i, F^t)$ that estimates y_i . To improve the estimations, another function of $F^{t+1} = F^t + h^{t+1}(x)$ is created so that h^{t+1} is as follows:

$$h^{t+1} = \operatorname{argmin}_{h \in H} EL(y, F^t) \tag{6}$$

where H Where H is the collection of candidate Decision Trees being considered for inclusion in the ensemble. Hence, the expected loss function could be defined as (Hancock and Khoshgoftaar 2020):

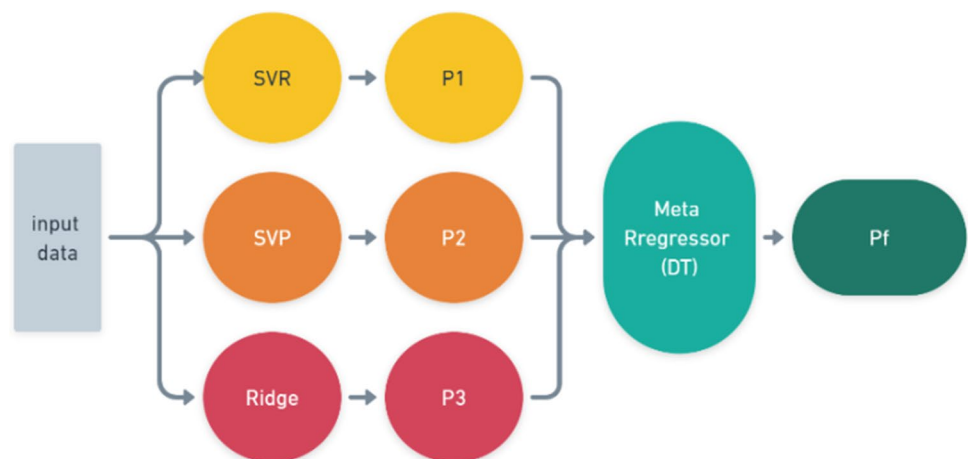
$$EL(y, F^{t+1}) = EL(y, F^t + h^{t+1}) \tag{7}$$

XGBoost

First introduced by Chen et al. (Chen and Guestrin 2016), extreme gradient boosting (XGB) is a variant of gradient boosting decision trees in which each base learner learns from the previous one to reduce its error. In general, the XGBoost technique builds a more robust aggregated model by combining many base learners (decision trees). Trees' weights are used in an XGBoost algorithm to approximate the final outcome. For each dataset with m characteristics, Eq. (8) is being used to forecast the outcome:

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), f_k \in \{f(x) = \omega_q(x)\} (q : R^m \rightarrow T, \omega \in R^T) \tag{8}$$

Fig. 5 Determined structure for the Stacked Regression model



Incorrectly defining the parameters of decision trees, such as their depth or number of iterations, may lead to overfitting. The XGBoost algorithm's excellent regularisation capabilities are what make it adequate. XGBoost penalizes models for overfitting by including and regularising approaches. XGBoost model optimization needs the tweaking of many hyperparameters. As the XGBoost method is a sort of ensemble and gradient boosting technique, its hyperparameters may be divided into four categories: ensemble hyper-parameters, tree hyper-parameters, sub-sampling hyper-parameters, and regularisation hyper-parameters (Tao et al. 2021).

CatBoost

Proposed by Prokhorenkova et al. (2018) is an improved version of the GBDTs. First, CatBoost handles high-cardinality categorical data better than Gradient Boosting. CatBoost employs one-hot encoding for low-cardinality categories. Besides, CatBoost benefits from the Ordered Boosting method. By assuming D as the set of all available data for training the GBDT model, and having in mind that the decision tree h^{t+1} is the tree that minimizes the loss function (L), Ordered Boosting could be expressed as using the same examples used for computation of Ordered Target Statistics for computation of h^{t+1} . Oblivious Decision Trees (ODTs) are a crucial component in CatBoost's method for constructing Decision Trees. CatBoost builds a collection of ODTs. ODTs are complete binary trees, hence if there are n levels, there will be $2n$ nodes. In addition, all non-leaf nodes in the ODT will use the same criterion for splitting. CatBoost extends GBDT's abilities so that it could account for feature interactions so that believe CatBoost will pick the most effective feature combinations throughout training (Prokhorenkova et al. 2018; Hancock and Khoshgoftaar 2020). CatBoost is highly sensitive to the definition of hyperparameters so a proper tuning of hyper-parameters would be essential.

Hyperparameter optimization

Optimization of hyper-parameters is an important task when it comes to automated machine learning (AutoML). AutoML automates complex operations, including model parameter optimization, without the need for human knowledge and so plays a crucial role in improving the performance of machine learning models (Tao et al. 2021). Bayesian optimization is a powerful method for figuring out the extreme values of computationally challenging functions. (Brochu et al. 2016). Additionally, it may be used to compute difficult-to-calculate, difficult-to-analyze derivatives, or nonconvex functions. By integrating the prior distribution of the function $f(x)$ with the sample data, Bayesian optimization makes the assumption

that it can utilize prior knowledge to determine where the function $f(x)$ is minimized in terms of a given criterion. The function u , also known as the acquisition function and serving as the criteria, is used to choose the next sample point in order to maximize predicted utility. It is necessary to take into account both seeking regions with high values (exploitation) and areas with high uncertainty (exploration) in order to decrease the number of samplings, which also increases accuracy (Wu et al. 2019). The prior distribution of the function f , which is mainly dependent on Bayesian optimization, is not always determined by objective criteria but may be partially or entirely determined by subjective judgements. Most people believe that the prior distribution used in Bayesian optimization matches the Gaussian process rather well. Bayesian optimization employs the Gaussian process to fit data and update the posterior distribution because it is flexible and easy to use (Wu et al. 2019).

In this study, Bayesian optimization is utilized to automatically tune the hyper-parameters of all models to estimate the discharge coefficient and through flow discharge. Best models are then reconstructed and used to calculate accuracy metrics. Figure 6 visualizes the relationship between hyper-parameters and the obtained accuracy for the XGBoost regression model during the performed optimization process. The hyper-parameters obtained from the optimization process for each model are presented in Tables 2 and 3.

Model development and accuracy assessment

All models are developed and implemented using Scikit-learn (DT, AdaB,RF) (Pedregosa et al. 2011), Mlxtend (Stacked reg.) (Raschka 2018), XGBoost library (Chen 2016–2022), and the CatBoost (LLC 2017–2022) library. Three accuracy measures are used to evaluate the accuracy of the utilized ensemble models, including Mean absolute error, Mean squared error and the correlation coefficient which are frequently used in similar research for regression tasks, i.e. see (Azimi et al. 2019) (Hameed et al. 2021).

Mean Absolute error (MAE):

$$\text{MAE} = \frac{\sum_{i=1}^n |y_i - \hat{y}_i|}{n} \quad (9)$$

Mean-squared error (MSE):

$$\text{MSE} = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n} \quad (10)$$

and the correlation coefficient (R^2):

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (11)$$

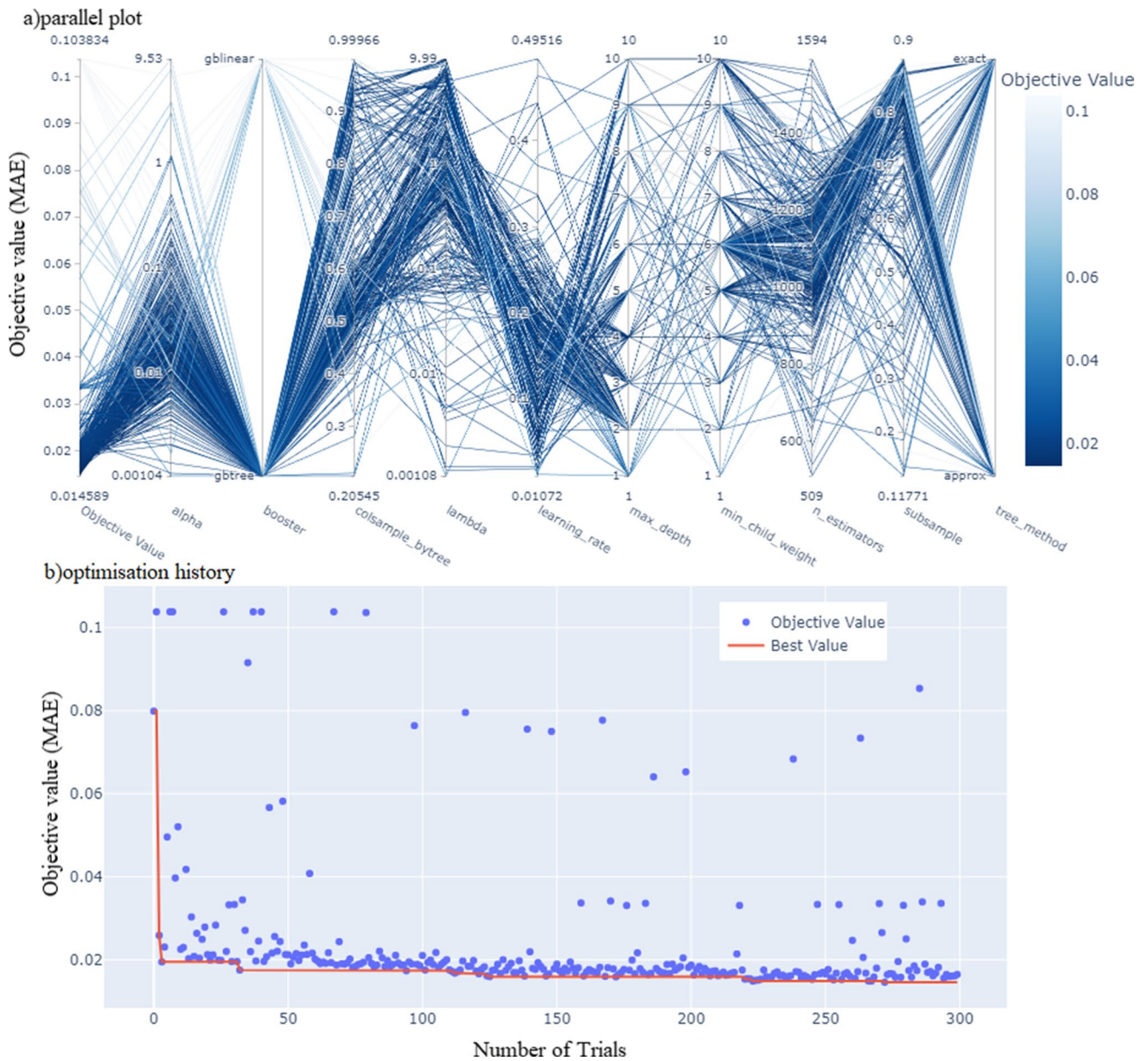


Fig. 6 Visualization of the hyper parameter optimization for the XGBoost regressor

Table 2 Utilized Hyper-parameters for base models

Model	SVR	SVP	DT
Hyper parameters	Kernel = RBF Coef0 = 0.44 tol = 0.01 ϵ = 0.028 C = 9	Kernel = poly Degree = 3 Coef0 = 0.51 tol = 0.051 ϵ = 0.025 C = 1	Splitter = best Max_depth = 25 Loss = MAE Min_leaf = 2 Min split = 2

The target value from experimental data \hat{y}_i is the model predictions and \bar{y} represents the mean values. Figure 7 presents the general workflow of the current paper.

Results and discussion

Feature importance and recursive feature elimination

Considering the sensitivity of models to the input data and features, the relative importance of input features for different algorithms to estimate the discharge coefficient C_d and the through-flow discharge ratio Q_{in}/Q_i are presented in Figs. 8 and 9, respectively. It could be concluded that the porosity (n) with the weak correlation of (-0.26) with the C_d , had a higher correlation than upstream and downstream slopes. Yet, its relative importance for all

Table 3 Utilized Hyper-parameters for ensembles

Model	GBDT	XGB	CatB	RF
Hyper parameters	Loss = Huber Criterion = MSE learning_rate = 0.1 subsample = 0.35 min_split = 2 min_leaf = 1 weight_fraction = 0.001 max_depth = 4 N_estimators = 300	n_estimators = 1200 max_depth = 2 subsample = 0.8759 colsample_bytree = 0.5094 alpha = .029 tree_method = approx booster = 'gbtree' min_child_weight = 6 lambda = 1.0794 learning_rate = 0.2	N_estimators = 2000 learning_rate = 0.042 depth = 5 l2_leaf_reg = 0.0045 loss = RMSE max_bin = 353 min_data_in_leaf = 223	Splitter = best Max_depth = 25 Loss = MAE Min_leaf = 2 Min_split = 2 N_estimators = 2300

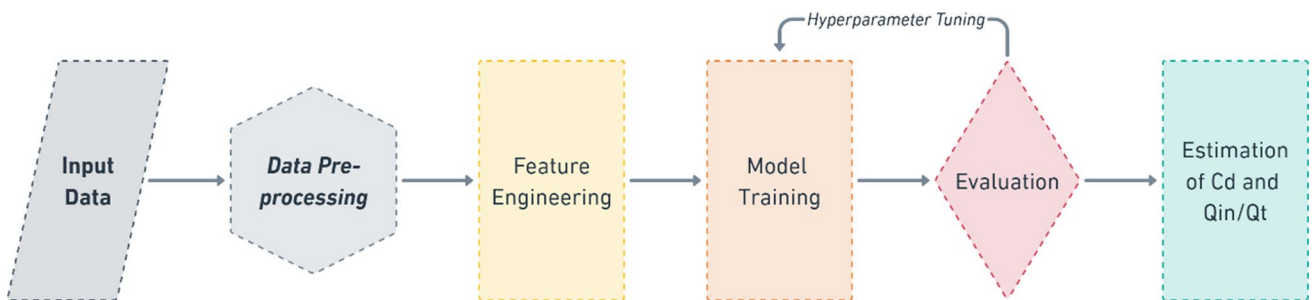


Fig. 7 model training workflow

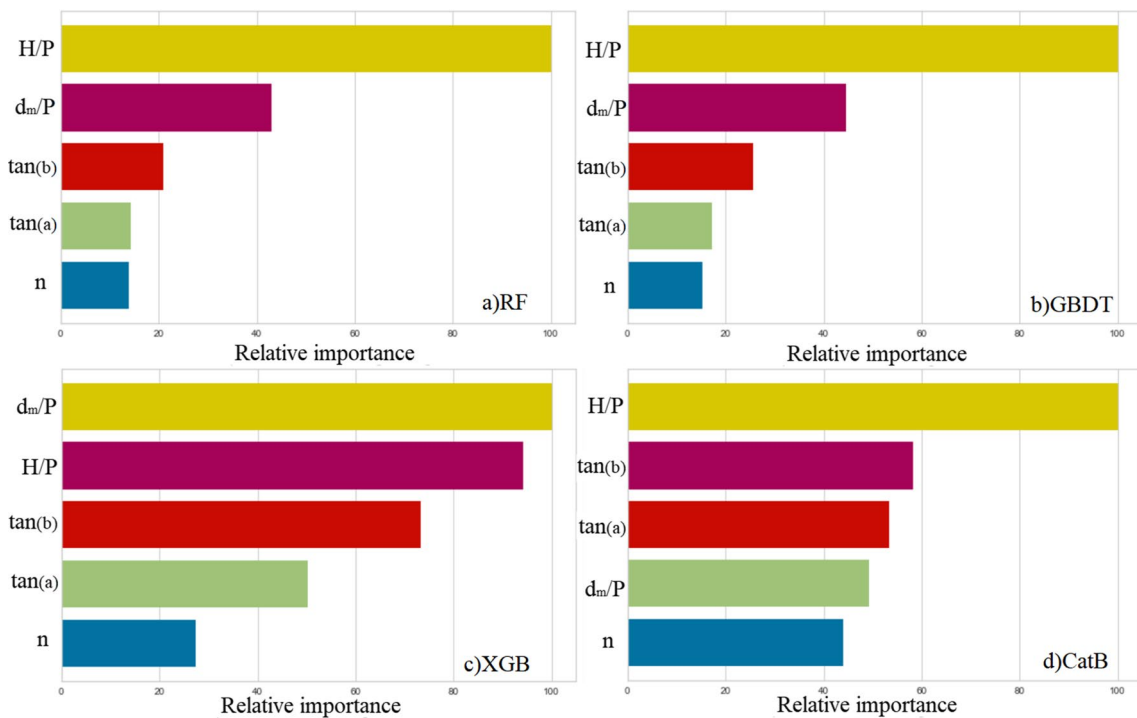


Fig. 8 Feature relative importance for estimation of C_d

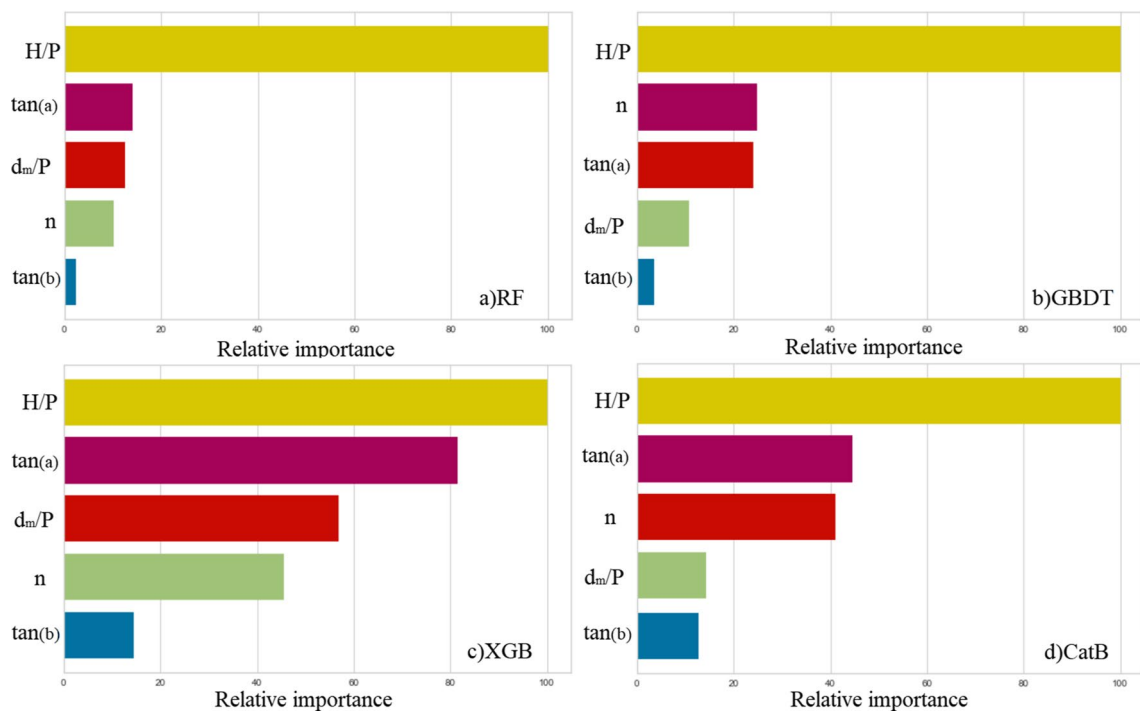


Fig. 9 Feature relative importance for estimation of Q_{in}/Q_t

regression models is the lowest among all the features. Besides, the relative flow head (H/P) and the relative particle size (d_m/P) have the highest relative importance for estimating C_d in all models except the CatBoost, in which the importance if downstream and upstream slopes are higher than that of d_m/P . Regarding models trained for estimation of Q_{in}/Q_t , the lowest importance of features belongs to the downstream slope $\tan(b)$ while the importance of porosity (n) is increased especially for CatBoost and GBDT models. Yet the most important feature is the

relative flow head (H/P). In order to investigate the effect of different feature combination on the models accuracy, a recursive feature elimination (RFE) test is performed for all models. Generally results indicate that models perform best when all features are included yet the only exception is GBDT which had higher accuracy with the 4 best features. Results of the RFE test for XGB are depicted in Fig. 10. Best models are then recreated and fitted on the training dataset combining the results of hyper parameter optimization and RFE test.

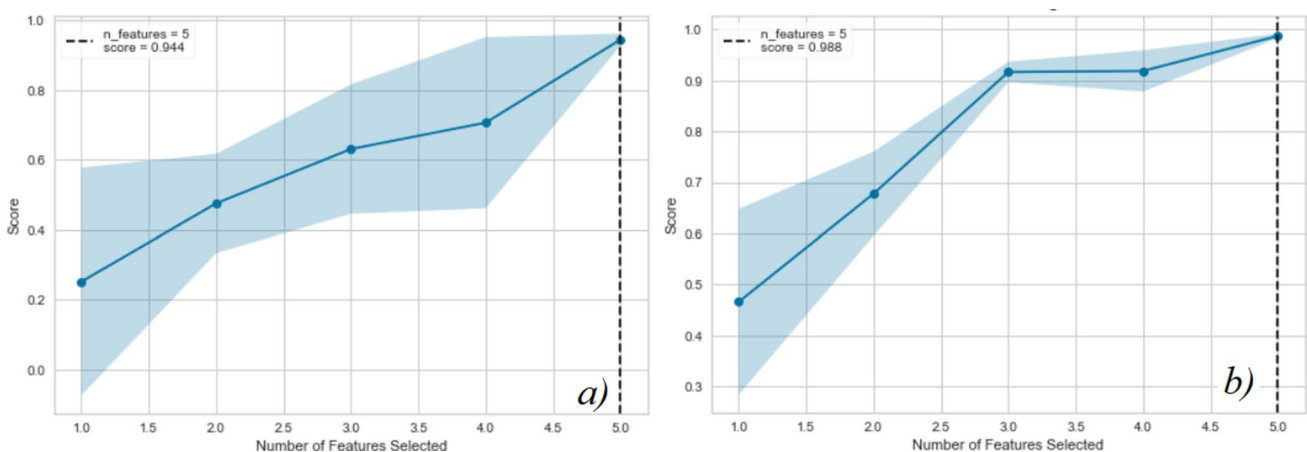


Fig. 10 Recursive Feature elimination analysis for XGB model for a C_d and b Q_{in}/Q_t

Table 4 Accuracy metrics of different algorithms in estimation of C_d

Model	Train		Test	
	R^2	R^2	MAE	MSE
SVR	0.977	0.962	0.0188	0.00067
SVP	0.968	0.931	0.0221	0.00122
DT	0.921	0.821	0.0432	0.00373
RF	0.940	0.912	0.0245	0.00171
Stacked	0.993	0.9643	0.0175	0.00062
GBDT	0.996	0.962	0.0187	0.00069
XGB	0.999	0.974	0.0147	0.00048
CatB	0.993	0.982	0.126	0.00033

Estimation of the discharge coefficient (C_d)

Based on the optimization results, the best models were then rebuilt and trained over the train-test dataset.

The results obtained from single and ensemble models in terms of their accuracy in predicting the discharge coefficient are presented in Table 4 and Fig. 11. It is indicated that the base DT model performs poorly in estimation of the discharge coefficient. Standalone support vector machine with RBF kernel (SVR) and the support vector model with a third degree polynomial kernel (SVP) models have shown proper performance of $R^2 = 0.96$ and 0.931 , respectively. Among ensemble models, the well-known Random forest (RF) model as a representative of bagging techniques has improved the accuracy of the based DT model by 9% showing an accuracy of $R^2 = 0.921$ and RMSE and MSE equal to 0.0245 and 0.00171 , respectively, while it is still lower than that of support vector machines. The stacking regression method composed of SVMs and the DT as meta-model however shows a higher $R^2 = 0.964$ with $MAE = 0.175$ and $MSE = 0.00061$ compared to the optimized GBDT model with $R^2 = 0.962$ and $MAE = 0.161$, and $MSE = 0.0061$. Consequently, the variance and the standard deviation of the residuals in the stacked model is higher than that of GBDT model despite its higher R-squared value. XGB and CatBoost offer higher accuracy among other models with $R^2 = 0.974$ and 0.982 , respectively. CatBoost outperforming the XGB in terms of all accuracy measures by 0.8% margin in R^2 value. Consequently, it could be concluded that even though the XGB model outperformed all other models, CatBoost has outperformed XGB considerably by increasing 1.2% the R^2 value and reducing MSE value for almost 31% .

Estimation of the through-flow discharge ratio (Q_{in})

The results obtained from single and ensemble models in terms of their accuracy in predicting the Q_{in}/Q_t ratio are presented in Table 5 and Fig. 12. Clearly, the poorest results obtained from Decision Tree model with $R^2 = 0.865$ and

Table 5 Accuracy metrics of different algorithms in the estimation of Q_{in}/Q_t ratio

Model	Train		Test	
	R^2	R^2	MAE	MSE
SVR	0.977	0.976	0.0141	0.00028
SVP	0.971	0.968	0.0154	0.00036
DT	0.983	0.865	0.0321	0.00159
RF	0.991	0.947	0.0219	0.00074
Stacked	0.997	0.978	0.0132	0.00025
GBDT	0.996	0.989	0.0087	0.00012
XGB	0.999	0.992	0.0079	0.000091
CatB	0.998	0.992	0.0071	0.000094

Random Forest with and $R^2 = 0.947$ and $MAE = 0.0219$. The SVP and SVR models have shown proper accuracy of $R^2 = 0.968$ and $R^2 = 0.976$, respectively, while the Stacking regression ensemble model has resulted in an accuracy of $R^2 = 0.978$ which could be considered a slight improvement of the performance of the base SVR model. GBDT model shows a significant performance improvement compared to other models with $R^2 = 0.989$, $MAE = 0.0087$ and $MSE = 0.00012$. Utilizing the XGBoost and CatBoost algorithms, which produced $MAE = 0.0079$ and 0.0071 and MSE of 0.000093 and 0.000094 , respectively, and may be deemed to have almost comparable performance, model accuracy is improved up to $R^2 = 0.992$.

Residuals and feature importance analysis

Residuals are the difference between the observed value of the dependent variable (y) and the expected value (\hat{y}). The residuals plot depicts the difference between residuals on the vertical axis and the dependent variable on the horizontal axis, aiding in the identification of error-prone areas of the target. The residuals of the different algorithms by means of estimation of the discharge coefficient C_d and the through-flow discharge ratio Q_{in}/Q_t are presented in Figs. 13 and 14, respectively. A comparison of the residuals shows that the distribution of residuals around the centreline for all models is fairly random, suggesting that the models have generalized well, yet the CatBoost model shows almost zero residual for the training phase, which could be considered as overfitting. It is also worth noting that the majority of errors arise from C_d values close or above 1 which represents the experiments with lower discharge and limited training data.

Model sensitivity analysis

Considering that the sensitivity analysis is an important step in each ML project, this paper studies the sensitivity

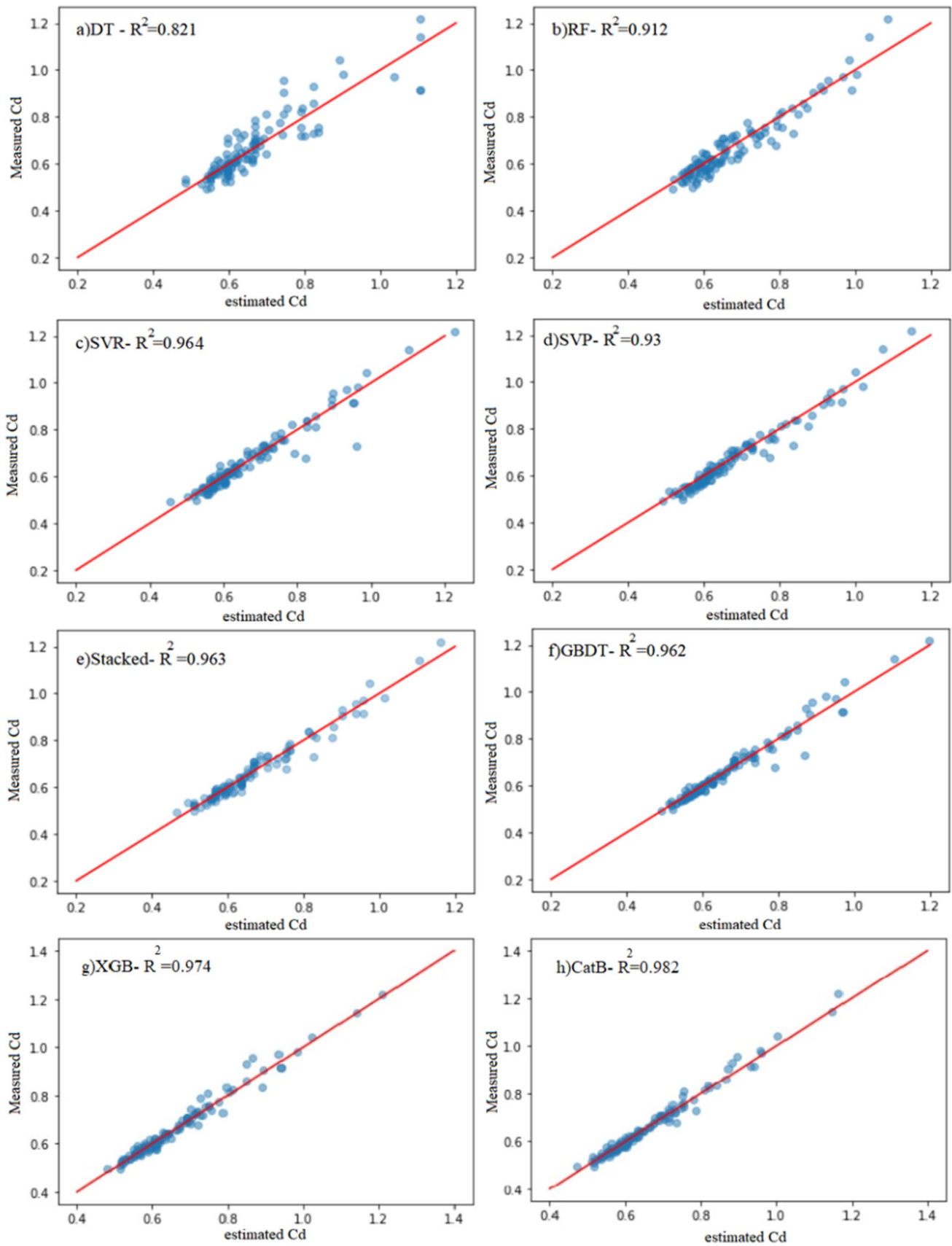


Fig. 11 Scatter plot of observed vs estimated values of C_d for different methods

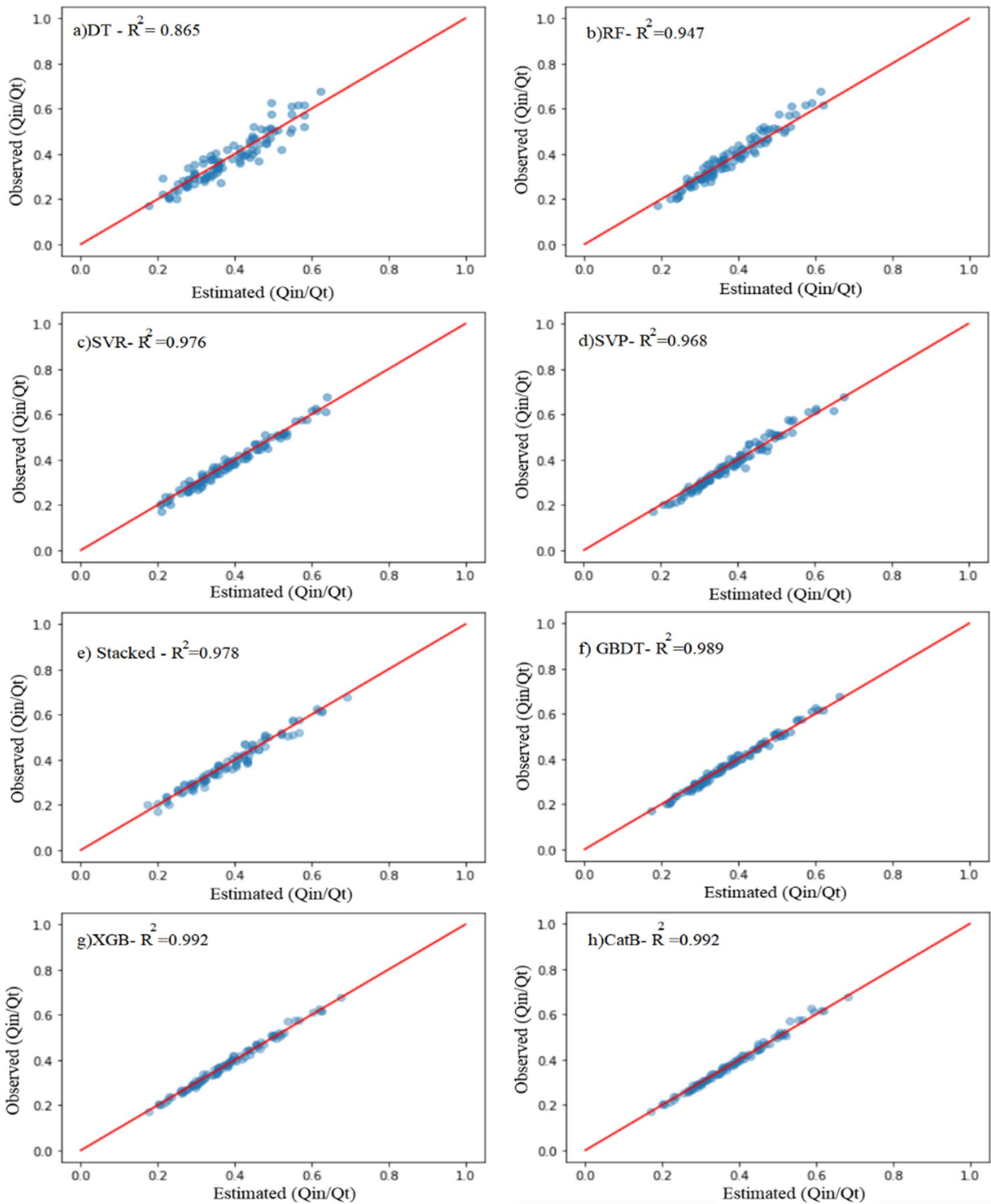


Fig. 12 Scatter plot of observed vs estimated values of Q_{in}/Q_t for different methods

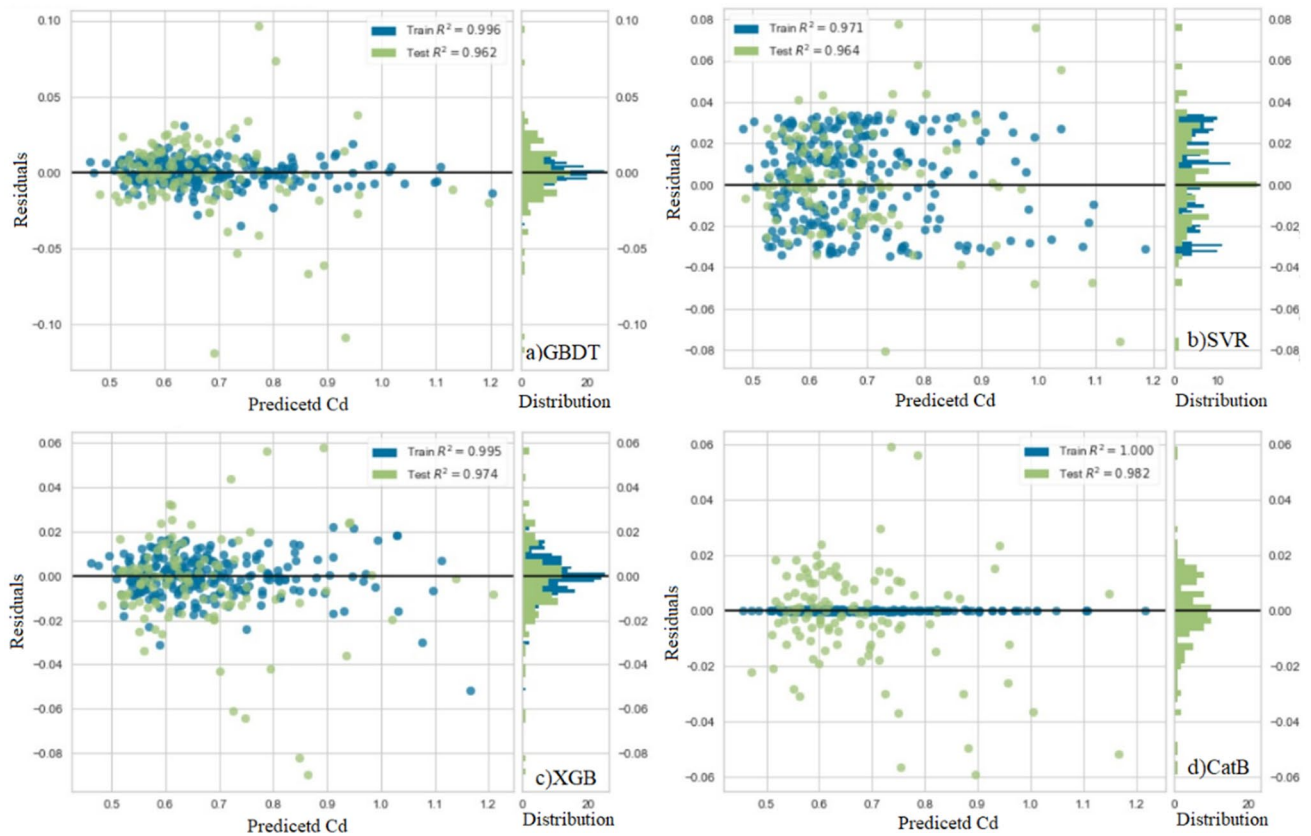


Fig. 13 Models residuals for estimation of C_d

of the top two models against the elimination of different features. Hence, at each step, one feature is eliminated and models are trained on the rest of the features. Obtained values of R^2 score are presented in Table 6. Results indicate that the most important features affecting the results are H/P, upstream slope and downstream slope. It should be noted that elimination of Reynolds number has increased the accuracy of CatB model to $R^2 = 0.994$ while it has reduced C_d values.

Conclusion

The current study makes use of some the well-known machine learning techniques such as Support vector machines, Decision trees(DT) and Random Forest (RF) models, as well as the stacking ensemble technique and three different Boosting ensemble models, including Gradient Boosting Decision Trees (GBDT), Extreme gradient Boosting model (XGB), and the more recent CatBoost model in order to evaluate the effectiveness of these models in estimation of the discharge coefficient (C_d) and the through-flow discharge ratio(Q_{in}/Q_t) of broad-crested gabion weirs. A

total of 368 data points from literature were extracted and used to train and evaluate the model's accuracy. The Bayesian optimization framework as well as the recursive feature elimination analysis are combined in order to improve the accuracy of the utilized ML models. Results indicate that the weakest performance with $R^2 = 0.82$ and 0.865 was obtained using the DT model to estimate the discharge coefficient and through flow discharge. The use of the stacking model improved the accuracy of base models to $R^2 = 0.9643$ and 0.978 for estimation of C_d and Q_{in}/Q_t , respectively. The maximum accuracy for estimating the discharge coefficient was achieved from the CatBoost model with $R^2 = 0.982$, MAE = 0.0126, and MSE = 0.00033. All boosting strategies produced accuracies higher than $R^2 = 0.962$ in terms of both the C_d and Q_{in}/Q_t estimation. Utilizing a sensitivity analysis for the top two models of XGBoost and CatBoost, a slight increase in performance of models was identified in terms of estimation of Q_{in}/Q_t ratio. While estimating the Q_{in}/Q_t values, CatBoost has outperformed other models including XGBoost slightly with $R^2 = 0.994$ against 0.922 of XGBoost model. Yet, the distribution of error residuals obtained from XGBoost is slightly better distributed, showing a slightly better performance in the model's generalisation.

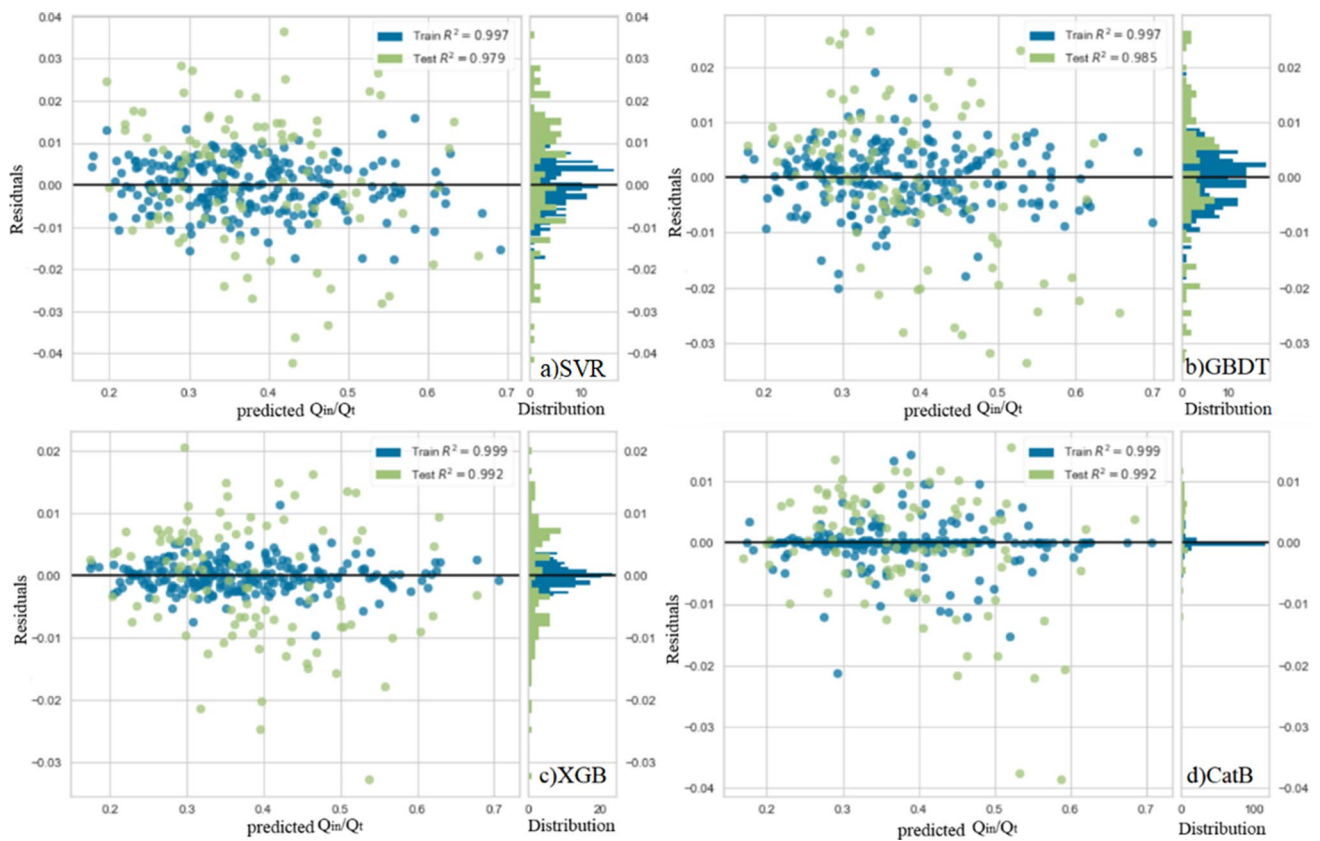


Fig. 14 Models residuals for estimation of Q_{in}/Q_t

Table 6 R^2 values resulted from sensitivity analysis of model results to features

	Eliminated feature	Tan(α)	Tan(β)	d_{50}/p	n	H/P	Re	d_{50}/p & n
C_d	CatB	0.781	0.707	0.981	0.975	0.652	0.980	0.764
	XGB	0.805	0.659	0.976	0.971	0.776	0.964	0.791
Q	CatB	0.702	0.938	0.992	0.990	0.702	0.994	0.761
	XGB	0.756	0.934	0.989	0.989	0.756	0.992	0.745

Acknowledgements Thank are due to all the authors for their contributions. All authors have read and agreed to the submitted version of the manuscript.

Funding The authors gratefully acknowledge the financial support from the National Natural Science Foundation of China (Grant Nos. 52179060 and 51909024).

Data availability The data that support the findings of this study are available from the corresponding authors upon reasonable request.

Declarations

Conflict of interest There is no conflict of interest in this manuscript.

Ethical approval

The author consents to participate in the works under the Ethical Approval and Compliance with Ethical Standards.

Ethical conduct

The principles of ethical and professional conduct have been followed.

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