Key Points:
- AI&DM approaches are useful tools to assist decision making in reservoir management
- A newly developed shuffled cross-validation scheme is robust against overfitting
- The enhanced CART algorithm is able to reproduce expert reservoir operation decisions

Simulating California reservoir operation using the classification and regression-tree algorithm combined with a shuffled cross-validation scheme

Tiantian Yang[1], Xiaogang Gao[1], Soroosh Sorooshian[1], and Xin Li[2]

[1]Department of Civil and Environmental Engineering, University of California, Irvine, California, USA, [2]Cold and Arid Regions Environmental and Engineering Research Institute, Chinese Academy of Sciences, Lanzhou, China

Abstract The controlled outflows from a reservoir or dam are highly dependent on the decisions made by the reservoir operators, instead of a natural hydrological process. Difference exists between the natural upstream inflows to reservoirs and the controlled outflows from reservoirs that supply the downstream users. With the decision maker's awareness of changing climate, reservoir management requires adaptable means to incorporate more information into decision making, such as water delivery requirement, environmental constraints, dry/wet conditions, etc. In this paper, a robust reservoir outflow simulation model is presented, which incorporates one of the well-developed data-mining models (Classification and Regression Tree) to predict the complicated human-controlled reservoir outflows and extract the reservoir operation patterns. A shuffled cross-validation approach is further implemented to improve CART's predictive performance. An application study of nine major reservoirs in California is carried out. Results produced by the enhanced CART, original CART, and random forest are compared with observation. The statistical measurements show that the enhanced CART and random forest overperform the CART control run in general, and the enhanced CART algorithm gives a better predictive performance over random forest in simulating the peak flows. The results also show that the proposed model is able to consistently and reasonably predict the expert release decisions. Experiments indicate that the release operation in the Oroville Lake is significantly dominated by SWP allocation amount and reservoirs with low elevation are more sensitive to inflow amount than others.

1. Introduction

Reservoirs and dams are the major infrastructures in California for surface water resources management, flood control, and ecosystem protection. Decision makers in California are under increasing pressure because of the emerging unsustainable water-supply problems caused by population growth, environmental degradation, and climate change. California's severe challenge of meeting rising water demands with limited resources has been widely recognized by decision makers after the state experienced the recent drought [*DWR*, 2013a, 2013b]. Such a changing situation brought the awareness of policy makers and water management agencies, such as the California Department of Water Resources (CDWR) and the U.S. Bureau of Reclamation (USBR), to timely establish and enforce water regulations and policies to promote water management efficiency in the vast reservoir systems in California. From the downstream water users' point of view, the amount of upstream inflows to reservoirs might not be sufficient information to establish proper water management plans for agriculture irrigation, ground water pumping, ecosystem protection, etc. To make efficient and prompt water planning, downstream users require a robust estimate on the actual amount water released from an upper-stream reservoir, which are expert release decisions by reservoir operators.

In order to estimate the controlled releases or storage, which are also termed as reservoir system yields, reservoir simulation models are widely used [*Louks and Sigvaldason*, 1981]. *Lund and Guzman* [1999] concluded that simulation models were more common in practice and, therefore, were more likely to be trusted as a standard compared to optimization models. In early times, *Sigvaldson* [1976] developed an innovative approach for simulating reservoir responses using a priority ranking concept. *Chaturvedi and Srivastava* [1981] developed a screen-simulation model using two types of linear programming methods for a large

complex water resources system. In the recent decades, many advanced reservoir simulation models were developed and became favored by many government agencies and research institutes, such as the HEC-5 simulation model developed by USACE [*Bonner*, 1989], DWRSIM developed by CDWR [*Barnes and Chung*, 1986; *Chung et al.*, 1989], the WEAP21 model [*Yates et al.*, 2005], the Calsim model [*Draper et al.*, 2004], etc.

As concluded by *Johnson et al.* [1991], the simulation models were only useful if the operating policies/rules incorporated in the simulation could realistically reflex the actual operation. In practice, reservoirs were always operated by so-called rule curves, which defined an empirically desired reservoir storage-release relationship [*Louks and Sigvaldason*, 1981]. However, *Oliveira and Loucks* [1997] pointed out that it was widely acknowledged that system operators often deviated from these rules to adapt to specific condition, objectives, or constraints that may exist at various times, even though the graphic rules provided a guidance for reservoir operation. *Draper et al.* [2004] also criticized that many simulation models were severally restricted by the complex coding of operating rules, which jeopardized the transparency to users. Therefore, in order to enhance the use of reservoir simulation models, it is of great importance of using suitable techniques to reproduce the actual release decisions and derive realistic and transparent reservoir operating policies/rules governed by both the traditional hydrological conditions (i.e., inflow, storage volume, precipitation, etc.) and many other nontraditional decision variables (i.e., water delivery and transfer, dry and wet conditions, downstream river stage, etc.).

To reach this goal, the attempts of using artificial intelligence and data-mining (AI&DM) techniques to simulate reservoir operation have gained much popularity. *Kuczera and Diment* [1988] developed a WASP (Water Assignment Simulation Package), which employed "What if" logic to explore the operating policy in a water transfer system. *Raman and Chandramouli* [1996] derived a general reservoir release rules using an artificial neural network algorithm. *Shrestha et al.* [1996] reconstructed the actual operation rules using a fuzzy-logic approach and compared the generated release with observation. *Rieker and Labadie* [2012] used a reinforced learning algorithm to simulate the long-term reservoir operation strategies in the Truckee River of California and Nevada. *Hejazi et al.* [2008] evaluated the sensitivities of hydrologic information's time scale and seasonality in reservoir historical releases in California and the Great Plain in U.S. *Corani et al.* [2009] used a Lazy Learning algorithm to reproduce human decisions in reservoir management in Lake Lugano. *Bessler et al.* [2003] extracted the operating rules for a single-reservoir in U.K. using the decision tree algorithm, linear regression and evolutionary algorithm, and found out that the results with decision tree algorithms were superior over the others. Compared among these three types of approaches, *Bessler et al.* [2003] also concluded that the decision tree algorithm had an advantage, which allowed the derived rules could be audited and further improved by domain experts. As it is compared to artificial neural network approaches, it is also believed that the simple Boolean logic used in decision tree approaches is more understandable to reservoir operators and easier to practice in real-world application.

Building on these previous works that focus on applying AI&DM techniques to reservoir management, in this study, we attempt to build a simple but efficient decision tree regression model to simulate controlled reservoir releases for nine major reservoirs in California, and investigate the impacts of multiple types of information on reservoir release decision making. In detail, three types of decision tree methods are tested and compared on nine major reservoirs in California, including the Classification and Regression Tree (CART) combined with a newly developed shuffled cross-validation scheme, the original CART algorithm with a standard twofold cross-validation scheme, and a benchmark Random Forest approach [*Breiman*, 2001].

The objectives of this study are to (1) develop a novel shuffled cross-validation scheme and jointly use with the CART algorithm, (2) apply the enhanced CART algorithm on nine reservoirs in California and compare with the original CART and Random Forest algorithms, and (3) evaluate the influences from multiple decision variables on reconstructing the expert reservoir decisions in California, including the daily releases, storage changes, and trajectories.

Compared to other pioneer studies, we extend the number of decision variables from only hydrological information's time scale and seasonality [*Hejazi et al.*, 2008] to 15 types of distinct information. Compared to *Corani et al.* [2009], in which high accuracy was achieved in reproducing human's decisions in a single lake in Italy, in this study, we aggressively attempt to reproduce the controlled outflow decisions in nine major reservoirs in California. The technique used in this study belongs to the same algorithm family that *Bessler et al.* [2003] employed but enhancement is introduced.
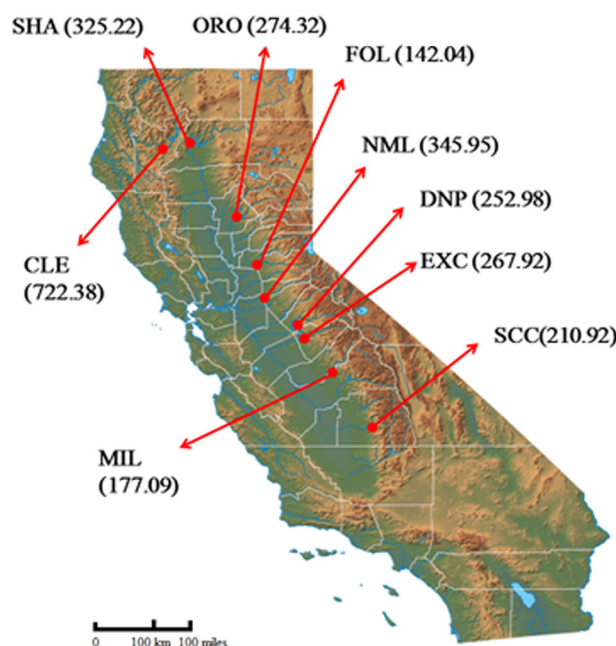
Figure 1. Locations of the selected reservoirs with elevations in parentheses (m).

This paper is organized into six sections: section 2 provides the information about the nine major reservoirs and the data used. The methodologies, including CART algorithm, Random Forest algorithm, shuffled cross-validation scheme, and Gini diversity index are introduced in section 3. Section 4 presents the simulation results of reservoir controlled outflows, storage daily changes, storage trajectories, and the sensitivity analysis on decision variables. Discussion, limitation, and future works are presented in section 5. Section 6 summarizes the conclusions and major findings.

2. Selected Reservoirs and Data

In this study, nine major reservoirs in California are selected, namely, the Trinity Lake, Don Pedro Reservoir, New Exchequer Reservoir, Folsom Lake, Friant Reservoir, New Melones Reservoir, Oroville Lake, Success Lake, and Shasta Lake. Most of the reservoir operation data and hydrological data are collected from the California Data Exchange Center (CDEC), which is an official data-sharing portal used by water agencies, decision makers, and water

Table 1. Basic Information for Selected Reservoirs, Snow Course Station, and Downstream River Gauges[a]

Name	River Basin	Station Type	ID	Latitude	Longitude	Elevation (m)	Agency	Function
Trinity Lake	Trinity	Res.	CLE	40.801	−122.762	722.4	USBR	WS, FC, EP Others
		S.C.	BBS	40.967	−122.867	1981.2	WRD	
		D.G.	DGC	40.645	−122.957	487.7	USGS	
Don Pedro Reservoirs	Tuolumne	Res.	DNP	37.702	−120.421	253.0	TID	FC, WS, Others
		S.C.	HRS	38.158	−119.662	2560.3	CDWR S/S	
		D.G.	MOD	37.627	−120.988	27.4	USGS	
New Exchequer Reservoirs	Merced	Res.	EXC	37.585	−120.270	267.9	MID	WS, FC, Others
		S.C.	STR	37.637	−119.550	2499.4	CDWR S/S	
		D.G.	CRS	37.425	−120.663	50.3	CDWR	
Folsom Lake	American	Res.	FOL	38.683	−121.183	142.0	USBR	WS, HP, Others
		S.C.	HYS	39.282	−120.527	2011.7	USBR	
		D.G.	AMF	38.683	−121.183	0.0	CDWR S/S	
Friant Dam	San Quaquin	Res.	MIL	37.001	−119.705	177.1	USBR	FC, WS, Others
		S.C.	NLL	37.257	−119.225	2438.4	SCE	
		D.G.	MEN	36.811	−120.378	51.8	USGS	
New Melones Reservoir	Stanislaus	Res.	NML	37.948	−120.525	346.0	USBR	WS, HP, FC, Others
		S.C.	BLD	38.450	−120.033	2194.6	USBR	
		D.G.	OBB	37.783	−120.750	35.7	CDWR	
Oroville Dam	Feather	Res.	ORO	39.540	−121.493	274.3	CDWR O/M	WS, FC, HP, EP, Others
		S.C.	KTL	40.140	−120.715	2225.0	CDWR O/M	
		D.G.	GRL	39.367	−121.647	28.0	CDWR O/M	
Success Dam	Tule	Res.	SCC	36.061	−118.922	210.9	USACE	FC, WS, Others
		S.C.	OEM	36.243	−118.678	2011.7	CAL FIRE	
		D.G.	TRL	36.087	−119.430	73.2	USACE	
Shasta Dam	Sacramento	Res.	SHA	40.718	−122.420	325.2	USBR	WS, HP, EP, Others
		S.C.	SLT	41.045	−122.478	1737.4	USBR	
		D.G.	IGO	40.513	−122.524	205.1	USGS	

[a]Res.: Reservoir; S.C.: Snow Course; D.G.: Downstream Gauge; WS: Water Supply; FC: Flood Control; HP: Hydropower; EP: Ecosystem Protection; Others: Navigation, Recreation, Groundwater Recharge, etc.; WRD: Weaverville Ranger District; CDWR S/S: CA Dept of Water Resources/Snow Surveys; USBR: U.S. Bureau of Reclamation; USACE: U.S. Army Corps of Engineers; TID: Turlock Irrigation District; MID: Merced Irrigation District; CDWR O/M: CA Department of Water Resources/O & M; SKCNP: Sequoia and Kings Canyon National Parks; SCE: Southern California Edison Company, Big Creek; USGS: US Geological Survey.

users in California. The CDEC installs, maintains, and operates a collection of extensive, centralized hydrologic operational, and historical data (http://www.water.ca.gov/floodmgmt/hafoo/hb/cdecs/) gathered from various agencies and utilities throughout the United States. Data supporting agencies include the National Weather Service (NWS), the U.S. Army Corps of Engineering (USACE), the U.S. Bureau of Reclamation (USBR), the U.S. Geological Survey (USGS), the California Department of Water Resources (DWR), the Sacramento Municipal Utility District (SMUD), Pacific Gas & Electric (PG&E), the East Bay Municipal Utility District (EBMUD), and multiple local water agencies. In addition, we retrieve the snow depth data and downstream flow information from each reservoir's nearby snow course station and river gauge station in the downstream service area, respectively. A summary of selected reservoir, snow course station, and downstream gauge is provided in Table 1. Figure 1 shows the corresponding locations of the selected major reservoirs in California.

The reservoir operation data are categorized into model input (decision variables) and output (target variables). We summarize the types of model inputs and outputs as follows:

1. The first type of model input is the reservoir storage volume, which is widely used by USACE in California as the guidance for reservoir releases. The relationship between releases and storage volumes or water levels is always represented as graphical charts termed as "rule curves," which represent the empirically desired reservoir operation criteria to meet water supply objective, flood control, and engineering constraints. It is worth to mention that in model training phase, the storage volume is intentionally lagged for one time step (1 day) for all experiments. It means that current release decisions are based on the initial storage of the day instead of the ending storage of that day, which is similar to the approach employed by *Raman and Chandramouli* [1996]. In the verification phase, current storage input is calculated by the mass-continuity function using the simulated releases on the previous time step (day).

2. The second type of model input primarily includes mostly the traditionally hydrological data for the daily reservoir operation, such as the reservoir daily inflow, the daily accumulated precipitation (point measurement), snow depth in reservoir's upstream mountain area, and the flow conditions in the downstream water supplying area.

3. The third type of model input is the wet/dry conditions. CDWR uses the Water Year Index (WYI) for the Sacramento Valley and the San Joaquin Valley to classify the water-supply conditions in a water year. In California, WYI is an important guideline for water planning and management [*DWR*, 2013b, 2009, 2005]. Officially, the WYIs are determined by the State Water Resources Control Board (SWRCB), which categorizes five types of water year: (1) wet, (2) above normal, (3) below normal, (4) dry, and (5) critical year. The calculation and classification examples for WYIs for the Sacramento Valley and the San Joaquin Valley are included in supporting information (SI) for interested readers.

4. Besides the WYIs, there are six different river indices commonly used in California, which are the operational climate predictors forecasted and calculated by CDWR Snow Survey office in the beginning of each water year. According to the communication with CDWR, these indices are also used by other water agencies as indicators for evaluating the climate conditions and operating their facilities for the entire state. More detailed information of these indices can be found in CDWR Snow Survey office. Generally, the calculation of these indices is based on a linear regression method using multiple weather information, ground-based measurements, and decades of experiences of on-site hydrologists. Namely, the six river indices are the Sacramento Valley's October–March runoff, April–July runoff, and water year total runoff sum and the San Joaquin Valley's October–March runoff, April–July runoff, and water year total runoff sum.

5. The fifth type of model input is the State Water Project (SWP) allocation amount. This variable partially represents the influence of policy or law changes related to water transferring and allocation, because the amount of water transferred by SWP must abide with the California Water Codes (laws), agreements, and water rights among multiple stakeholders, and water agencies. In California, the SWP is designated to provide specific amounts of agricultural and municipal water supplies to its 29 agencies over the entire state. However, based on California's current water-supply condition, the SWP water supply is subject to change over time. Once a change of the projected water supply is authorized by the governor and the SWRCB, the 29 agencies can only receive and use the officially announced amount of water under jurisdictional rights, unless further announcement is released. For example, on 31 January 2014, the CDWR announced an amendment to the SWP allocation, in which the SWP allocation to farmers and

Table 2. Detailed Information on the Decision and Target Variables

Decision/Target Variable Names	Unit	Resolution
Reservoir daily initial storage	m^3	Daily
Reservoir inflow	m^3/d	Daily
Accumulated precipitation	mm/d	Daily
Downstream daily mean flow or river stage	m^3/d or m	Daily or 6 h
Snow depth	m	Daily or Monthly
Month of a year		Monthly
Sacramento Valley October–March runoff		Annually
Sacramento Valley April–July runoff	m^3	Annually
Sacramento Valley water year total runoff sum	m^3	Annually
Sacramento Valley Water Year Index (WYI)		Annually
San Joaquin Valley October–March runoff	m^3	Annually
San Joaquin Valley April–July runoff	m^3	Annually
San Joaquin Valley water year total runoff sum	m^3	Annually
San Joaquin Valley's Water Year Index (WYI)		Annually
SWP allocation announcement		Occasionally
Reservoir outflow (target variable)	m^3/d	Daily

agricultural water agencies is dropped to 0% due to continuing drought conditions in California. This change of regulation is enforced by California Governor Brown's drought declaration made on 17 January 2014. The infrastructures in California were operating under this action until another announcement was made on 18 April 2014, increasing the SWP allocation back to 5%. These changes in the allocation percentages as a result of the governor's announcements are retrieved from the California Water Control Board and the SWP official document archive.

6. The last model input concerns the influence of seasonality on reservoir operation, which is the month of a year.

7. The model output (target variable) is the controlled reservoir daily outflow.

Most of the data for the selected reservoirs cover 16 years from 1 October 1997 to 31 December 2013, except the Trinity Lake (CLE), New Exchequer Reservoirs (EXC), and Shasta Lake (SHA), of which the data start on 24 March 2003, 30 March 1999, and 1 January 2001, respectively. A summary of the decision variables and target variable is provided in Table 2.

3. Methodology

3.1. Classification and Regression-Tree (CART) Algorithm

The method we employ is a white-box and tree-like data-mining technique, termed the Classification and Regression Tree (CART) algorithm, combined with a novel shuffled cross-validation scheme. CART was originally introduced by *Breiman et al.* [1984], and further developed by *Breiman* [1996, 2001] into bagging-tree and random forest, respectively. Given a set of decision variables (inputs or predictor) and target variables (outputs), the mechanism in CART is to repeatedly find a classification of the target variable associated with its decision variables based on selected splitting rules so that any new prediction will be the most similar to its observation in terms of the splitting rule defined measurement. The classification tree will eventually divide the whole training data set space into multiple classes (leaves). Each class consists of a set of rules that splits the decision variable spaces. The regression tree takes the average of the target variable values in each class and stores the corresponding splitting rules. Once a new set of decision variable is given to the regression tree, an estimated target value will be returned following the stored splitting rules. In this study, the regression tree is primarily used.

Mathematically, CART is a nonparametric data-mining algorithm capable of predicting continuous dependent variable (target variable, $\vec{y} = R^m$) with categorical and continuous predictor variable (decision variables, $\vec{x} = R^n$). CART uses a binary tree to recursively partition the decision variable space into subsets in which the distribution of target variable is successively more homogenous [*Chipman et al.*, 1998]. Before each split in CART, the prior data set is called "parent" node and the two split sub-data sets are referred to "children" nodes. The partitioning procedure searches through all values of the decision variable $\vec{x}$ to find the variable $\vec{x}_{j \in n}$ that provides the best partition of the target variable $\vec{y}$ by maximizing the homogeneity of target variable $\vec{y}|\vec{x}_i \leq \vec{x}_j$ and $\vec{y}|\vec{x}_i > \vec{x}_j$ in the "child" nodes [*Razi and Athappilly*, 2005]. The maximum of homogeneity

is governed by the selected splitting rule, such as to minimize the summation of relative errors in "child" nodes (equation (1)) [*Hancock et al.*, 2005].

$$\arg \min \left(RE(d) \right) = \arg \min \left(\sum_0^L (y_l - \bar{y}_L)^2 + \sum_0^R (y_r - \bar{y}_R)^2 \right) \tag{1}$$

where y_l and y_r are the left and right "child" nodes with L and R numbers of target variables, $\bar{y}_L$ and $\bar{y}_R$ are the mean of resulting target variables in the left and right "child" nodes, and d is the decision or splitting rule governing the partition of the data the decision variable $\vec{x}$. The resulting "child" nodes are recursively partitioned into smaller subnodes until preset stopping criteria are met in the tree-growing procedure. The stopping criteria could be number of iteration, minimum number of samples in final "child" nodes (classes or leaf), or/and maximum of decision tree depth (size). In this study, the minimum number of samples in a leaf is set to 10, the maximum size of decision tree is set to 20, and number of iteration is set to be relaxed.

CART has many advantages which could be suitable for reservoir operation and favored by decision makers. The nature of data-driven mechanism of decision tree model provides the transparency in its model framework, which allows decision maker to audit and improve the simulation quality [*Bessler et al.*, 2003]. CART is a nonparametric algorithm, in which the simple Boolean logic used in each split is able to provide reasonable physical interpretation of historical data. Moreover, the CART algorithm is computationally efficient [*Breiman et al.*, 1984; *Lewis*, 2000]. The low cost computation characteristic is able to bridge modeling framework with the increasing amount of data in the so-called era of "big data."

The applications of CART algorithm, bagging-tree, and random forest are numerous in literature. *De'ath and Fabricius* [2000] employed CART in analyzing ecological data. *Lewis* [2000] applied CART in developing clinical decision rules. *Prasad et al.* [2006] used bagging-tree and random forest in ecological prediction. The use of CART algorithm is also very popular in many other fields, such as finance engineering [*Fayyad et al.*, 1996], system-failure detection [*Chebrolu et al.*, 2005], ecosystem modeling [*Araújo and New*, 2007; *Elith and Leathwick*, 2009], remote-sensing data analysis [*Xu et al.*, 2005], and reservoir operation [*Bessler et al.*, 2003; *Kumar et al.*, 2013a, 2013b; *Li et al.*, 2014; *Sattari et al.*, 2012; *Wei and Hsu*, 2008]. *Steinberg and Colla* [2009] and *Wu et al.* [2008] also summarized that CART is one of the top 10 algorithms in the field of data mining.

3.2. Random Forest

To obtain a good predictive performance, the output classes (tree leaves) have to be high. However, the risk of overfitting the observed data will accordingly increase. One mean to resolve this weakness is to use an ensemble method, such as bagging [*Breiman*, 1996], boosting [*Freund and Schapire*, 1996], random forest [*Breiman*, 2001] etc. Large-scale empirical comparison has been conducted by *Caruana and Niculescu-Mizil* [2006], in which the Random Forest algorithm achieved excellent performances compared to numerous supervised learning algorithms. According to *Liaw and Wiener* [2002], differs from the standard trees, each node is split using the best among a subset of predictors randomly chosen at that node, instead of all decision variables. This counterintuitive strategy turns out to perform very well compared to many other classifiers, including discriminant analysis, support vector machines, and neural networks, and is robust against overfitting [*Breiman*, 2001]. Therefore, in this study, Random Forest algorithm is also employed as a benchmark algorithm for comparison. Experiments are carried out comparing the observed controlled outflows with the results from random forest, the CART algorithm combined with a shuffled cross-validation scheme, and a standard CART algorithm with twofold cross validation as control run on nine major reservoirs in California. Some settings for the use of random forest are listed as follows: the number of trees in a forest is set to be 200; the number of variables in the random subset at each node is set to be 10; and the minimum of samples in a leave is 1 with the purpose of obtaining a fully developed tree.

3.3. Shuffled Cross-Validation Scheme

A major issue may arise when using the CART model on the data that contain significant random noises. This issue is termed as "overfitting" [*Breiman et al.*, 1984], in which any statistical model, such as the CART algorithm, tends to give a very good or near "perfect" fitting to the training data instead of an accurate estimate of the relationship between the target and decision variables, resulting in a poor predictive capability on a model "unseen" data. To overcome this problem, model ensemble approaches are commonly used in the decision tree algorithms, such as the strategy adopted in Random Forest [*Breiman*,

2001]. Using the model ensemble approach, the weak learners associated with poor predictive performances are constantly eliminated in the tree growing process. Different from the model ensemble approach, in this study, we attack the "overfitting" problem of CART by shuffling the training data, and maximizing the posterior performances to select the best model structure, i.e., the decision tree depth. The attempt is to efficiently use limited data to ensure a sufficient number of training samples that contain distinct information which are recognizable to the CART algorithm so that accurate predictions on any unseen data can be stabilized.

In order to achieve such a goal, we develop a shuffled cross-validation scheme and jointly use with the CART algorithm. The cross-validation scheme, also called the rotation estimation [*Bauer and Kohavi*, 1999; *Geisser*, 1975, 1993], is a model-validation technique for evaluating predictive performance of a statistical model on an independent or unseen data set [*Arlot and Celisse*, 2010; *Breiman et al.*, 1984; *Burnham and Anderson*, 2002; *Picard and Cook*, 1984]. Several commonly used methods are the hold-out method, the K-fold method [*Breiman and Spector*, 1992; *Kohavi*, 1995], and the leave-one/p-out cross-validation method [*Allen*, 1974; *Geisser*, 1975; *Stone*, 1977]. In this section, we introduce the shuffled cross-validation scheme. Generally, the concept is to randomly shuffle the training data and break the training data structure to ensure that the training data set contains even data points that represent all kinds of conditions, such as the operations in dry, wet, and normal years. Different from the random forest concept that the decision variables are randomly selected in developing each individual tree, the proposed scheme first creates many CART models using full decision variables but detects the weak learner (model with poor predictive performances) based on the posterior maximum likelihood of model performances on a prepartitioned data sets from the training data sets. In addition, there is no ensemble of multiple trees in the proposed scheme and only one final tree is built using CART algorithm.

Using the proposed scheme, the CART algorithm is iteratively used to develop many decision tree models with different model structures (tree depths). In addition, data are repeatedly shuffled by many times to create many independent training, validating, and testing data sets. The performances of these decision trees on the different shuffled training data sets are evaluated by the Nash-Sutcliffe model-efficiency coefficient [*Nash and Sutcliffe*, 1970] and stored in an archive. The reasons that we use the Nash-Sutcliffe model-efficiency coefficient are (1) the Nash-Sutcliffe model-efficiency coefficient is a popular measure of the accuracy in evaluating decision tree models [*Arlot and Celisse*, 2010; *Burnham and Anderson*, 2002; *Picard and Cook*, 1984], and (2) it is a normalized index that addresses the differences between simulation and observation. The commonly used RMSE criterion may not be the appropriate measure given the magnitudes of outflows that can vary significantly depending on the size of the reservoirs in the system. Then, a maximum-likelihood method is employed to select the best decision tree model according to model's predictive performances on a temporary hold-out data set within the whole training data set. The best model is further used to predict the reservoir controlled releases on the test data set, which model never sees during the training and validating period. The purpose of using maximum-likelihood method is to prevent model from giving a nonreproducible good prediction on one single shuffled training data set, especially when the shuffled training data set happens to have similar hydrological conditions with the validating data set.

In order to further illustrate the mentioned shuffled cross-validation scheme, a detailed procedure is listed as: (1) the data are split into a training set and a test set, which is identical to the hold-out method. The training set includes about 80% of the data, and the test set includes the remaining data; (2) the training data set is then shuffled and further split into two subsets, with the first subset containing about another 80% of the training data and the second one containing the remaining data; (3) we iterate one of the structural parameter of CART (decision tree depth) from (2) to user-defined maximum and build a corresponding decision tree model using the first subset; (4) the Nash-Sutcliffe model-efficiency coefficient has been calculated for each model using the second subset; (5) the model with the highest Nash-Sutcliffe model-efficiency coefficient is selected, and the corresponding decision tree depth has been stored; (6) the processes of (2)–(5) are repeated for many times (e.g., 50,000 iterations), and the possibility functions of the numbers of candidate models in each tree depth are obtained; (7) the best decision tree depth is chosen based on the highest likelihood of the numbers of candidate models falling into each tree depth; (8) the verification experiment is carried on using the hold-out data set from Step (1). The flowchart of this shuffled cross-validation scheme is shown in Figure 2.
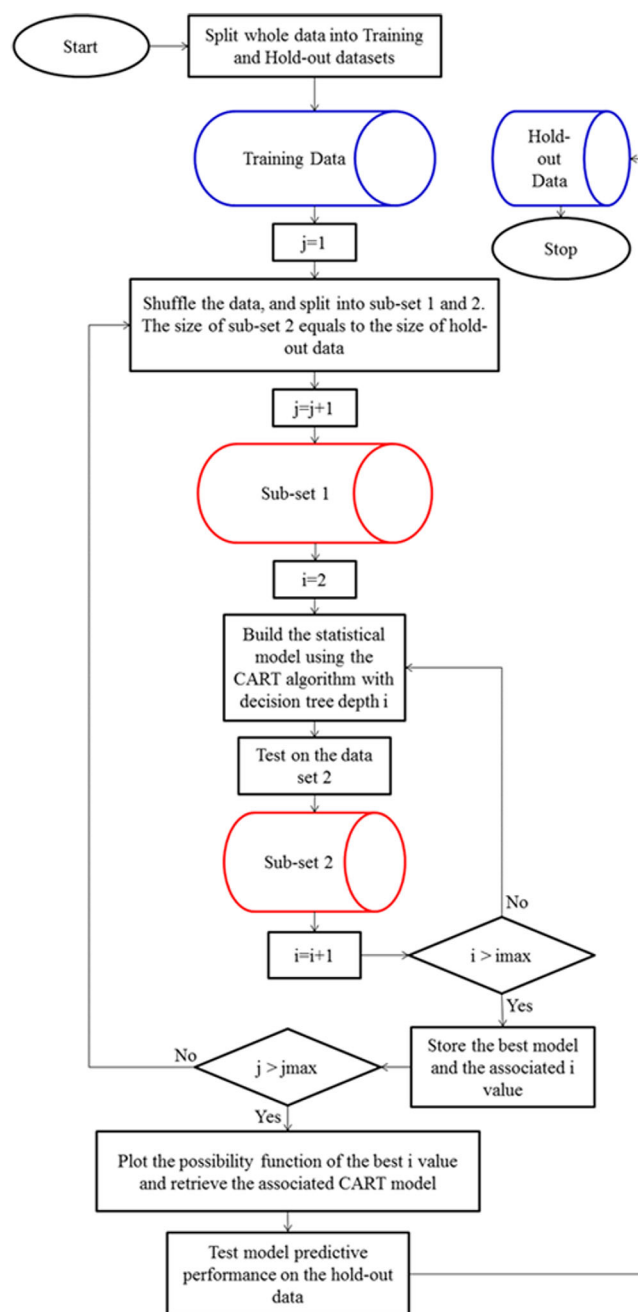
Figure 2. Flowchart of the shuffled cross-validation scheme.

The proposed scheme differs from the cross-validation methodology. The scheme combines the strength of (a) the hold-out methodology, (b) the K-fold method that, in our scheme, K approximately equals to 2, and the data used for training are about 60% of the whole data sets, (c) the leave-p-out method in which the training data set is shuffled and left about 20% of the training data set out, and (d) the maximum-likelihood estimation. The main purpose of combining these techniques is to ensure that the training data contain the proper predictabilities so that the selected model is able to utilize the historical information in predicting any model "unseen" (independent) data.

3.4. Gini Diversity Index

In the decision tree growing stage, as the same to all decision tree family, CART relies on the splitting rule that measures how well a split will result in the most homogenous "child" nodes. Two types of splitting rules, namely, the Gini index of diversity criterion and Twoing criterion, are originally introduced by *Breiman et al.* [1984]. The Gini diversity index is a standard and broadly used rule in CART. According to *Breiman et al.* [1984], the Gini diversity index measures the impurity of a node, while the Twoing criterion chooses a split that balances the data sets in the "child" nodes, which is not related to a node impurity measure. The use of Gini diversity index in CART is also favored by many researchers in the feature selection problem [*Chandra et al.*, 2010; *Guyon and Elisseeff*, 2003; *Qi et al.*, 2006; *Sandri and Zuccolotto*, 2008, 2010] , as well as in the field of reservoir operation [*Tsai et al.*, 2012; *Wei*, 2012]. Following these previous works, in this study, we also adopt Gini diversity index as the splitting rule in CART and use it as the measure to quantify decision variable's contribution. According to *Timofeev* [2004], Gini diversity index is calculated by the impurity function $i(t)$ shown in the following equation (2):

$$i(t) = \sum_{k \neq l} p(k|t)p(l|t) \qquad (2)$$

where $k, l \in 1, 2, \ldots, K$ are the index of the class (leaves); $p(k|t)$ is the conditional probability of class k provided that is in node t. The maximization of homogeneity of all child nodes will be equivalent to maximization of change of impurity function $\Delta i(t)$, as shown in equation (3):

$$\arg\max\left(\Delta i(t)\right) = \arg\max\left[-\sum_{k=1}^{K}p^2(k|t_p) + P_l\sum_{k=1}^{K}p^2(k|t_l) + P_r\sum_{k=1}^{K}p^2(k|t_r)\right] \tag{3}$$

where t_p, t_l, and t_r are the parent, left "child," and "right" child nodes, respectively; P_l and P_r are the probability of left "child" and right "child" nodes, respectively.

The details of other splitting rules and measurements are available in literatures, such as the Twoing rules [*Breiman et al.*, 1984], the Quinlan's information gain measure (IM) [*Quinlan*, 1979, 1986], Marshall Correction [*Mingers*, 1989], and a random selection of attribute for splitting. The comparisons of different measures are also numerous, such as the works by *Mingers* [1989] and *Buntine and Niblett* [1992].

4. Results

In this section, experiment settings and simulation results are demonstrated. The simulated reservoir controlled outflows are compared with observation under three different scenarios, including CART combined with shuffled cross-validation scheme, original CART with twofold cross validation, and random forest. Using the simulated controlled outflows, reservoir daily storage changes and storage trajectories are further calculated. The contributions of decision variables from different methods are compared using the Gini diversity index.

4.1. Experiment Settings

As introduced in section 2, though the data lengths for the nine major reservoirs in California (Table 2) are not same, most of them are from 1 October 1997 to 31 December 2013. Based on a commonly accepted "80/20" split rule, we hold out the data from 1 January 2010 to 31 December 2013 as test period and the rest are used for training and cross validation. In the shuffled cross-validation scheme, the tree depth for each iteration are set from 2 to 20 and the training data are shuffled 50,000 times, as shown in section 3.3: Steps (2)–(5). This means that there are 700,000 $((15 - 2 + 1) \times 50,000)$ candidate decision tree models being constructed and validated using the shuffled training data. The Nash-Sutcliffe model-efficiency coefficient is calculated to evaluate the model performance and compare the candidate models. There are total 19 CART models with tree-depth parameters ranging from 2 to 20 are constructed using 50,000 shuffled training data sets, but not all of the models are qualified to be the candidate model. In each shuffle, one candidate model is obtained by selecting the best one among the 19 CART models. Therefore, after 50,000 shuffles, a total of 50,000 candidate models are created, which fall into 19 types of CART models. Each type of tree contains certain numbers of the candidate model. Figure 3 plots the frequency histograms of candidate models in the 19 types of CART models applied to California major reservoirs (CLE, DNP, EXC, FOL, MIL, MNL, ORO, SCC, and SHA) using the shuffled cross-validation scheme (red). The best depth for decision tree models applied to the reservoir has the maximum frequency, which indicates that this type of decision tree model is expected to have the most stable and accurate predictive performance on the "unseen" data. The selected depths for reservoirs CLE, DNP, EXC, FOL, MIL, MNL, ORO, SCC, and SHA are 12, 14, 13, 11, 13, 9, 9, 12, and 15, respectively. In Figure 3, the frequency histogram of using CART with a standard twofold cross validation is also shown. The corresponding maximum of the best tree depths for the nine reservoirs are 9, 12, 8, 8, 8, 6, 7, 7, and 9, respectively. A slightly higher tree depth and larger size of tree are chosen when using the shuffled cross-validation scheme. With regard to random forest, the final depths from one random candidate tree are 24, 24, 26, 31, 25, 28, 26, 29, and 29 for the nine reservoirs, respectively.

4.2. Simulation Results for Controlled Outflows, Storage Changes, and Trajectories

Using the selected decision tree depths from the previous section, we test the predictive capability of the decision tree model on the hold-out data set (31 December 2010 to 31 December 2013). The purpose is to examine the actual model's predictive performance. Because the hold-out data are never used in any training process, here they are considered as an independent future scenario. The closer the predicted outflow to the observation, the better predictive performance the model has. The predicted daily outflows from the nine major reservoirs in California are shown in Figure 4.

To mathematically quantify and compare models' performance, we chose four statistical measurements suggested by *Gupta et al.* [1998], namely, Root-Mean-Square-Error (RMSE), correlation coefficient (R), Nash-Sutcliffe Model Efficiency (NSE), and Peak Flow Difference (PDIFF). In Table 3, the computed statistics for
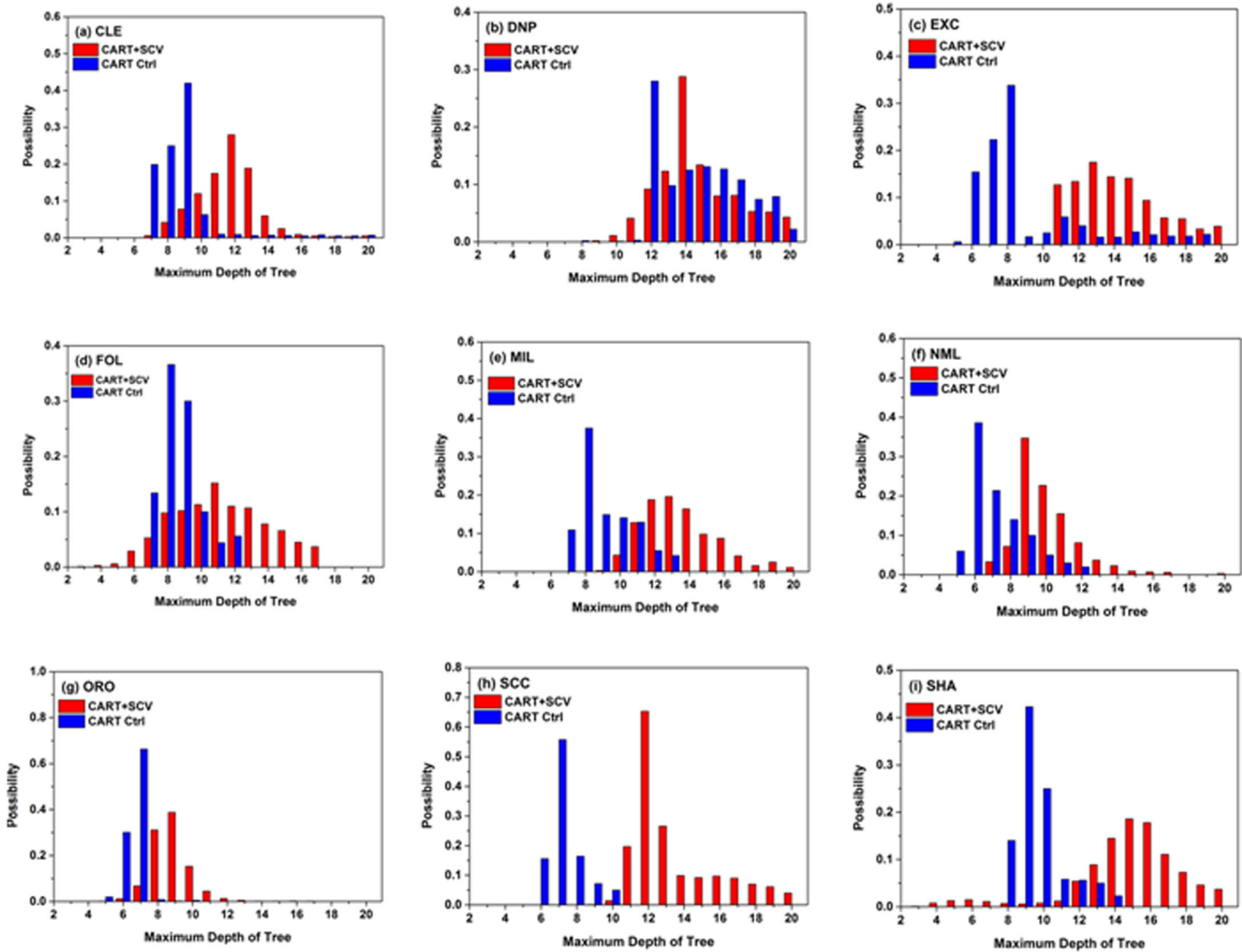
Figure 3. The frequency histograms of CART tree depths using both shuffled cross validation and standard twofold cross validation for the selected nine major reservoirs in California.

nine reservoirs' controlled outflows simulation are summarized. The formula for calculating the selected statistical measurements are listed as follows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(Q_{obs,i}-Q_{sim,i})^2}{N}} \tag{4}$$

$$R = \frac{\sum_{i=1}^{N}(Q_{obs,i}-\bar{Q}_{obs,i})(Q_{sim,i}-\bar{Q}_{sim,i})}{\sqrt{\sum_{i=1}^{N}(Q_{obs,i}-\bar{Q}_{obs,i})}\sqrt{\sum_{i=1}^{N}(Q_{sim,i}-\bar{Q}_{sim,i})}} \tag{5}$$

$$NSE = 1 - \frac{\sum_{i=1}^{N}(Q_{obs,i}-Q_{sim,i})^2}{\sqrt{\sum_{i=1}^{N}(Q_{obs,i}-\bar{Q}_{obs,i})}} \tag{6}$$
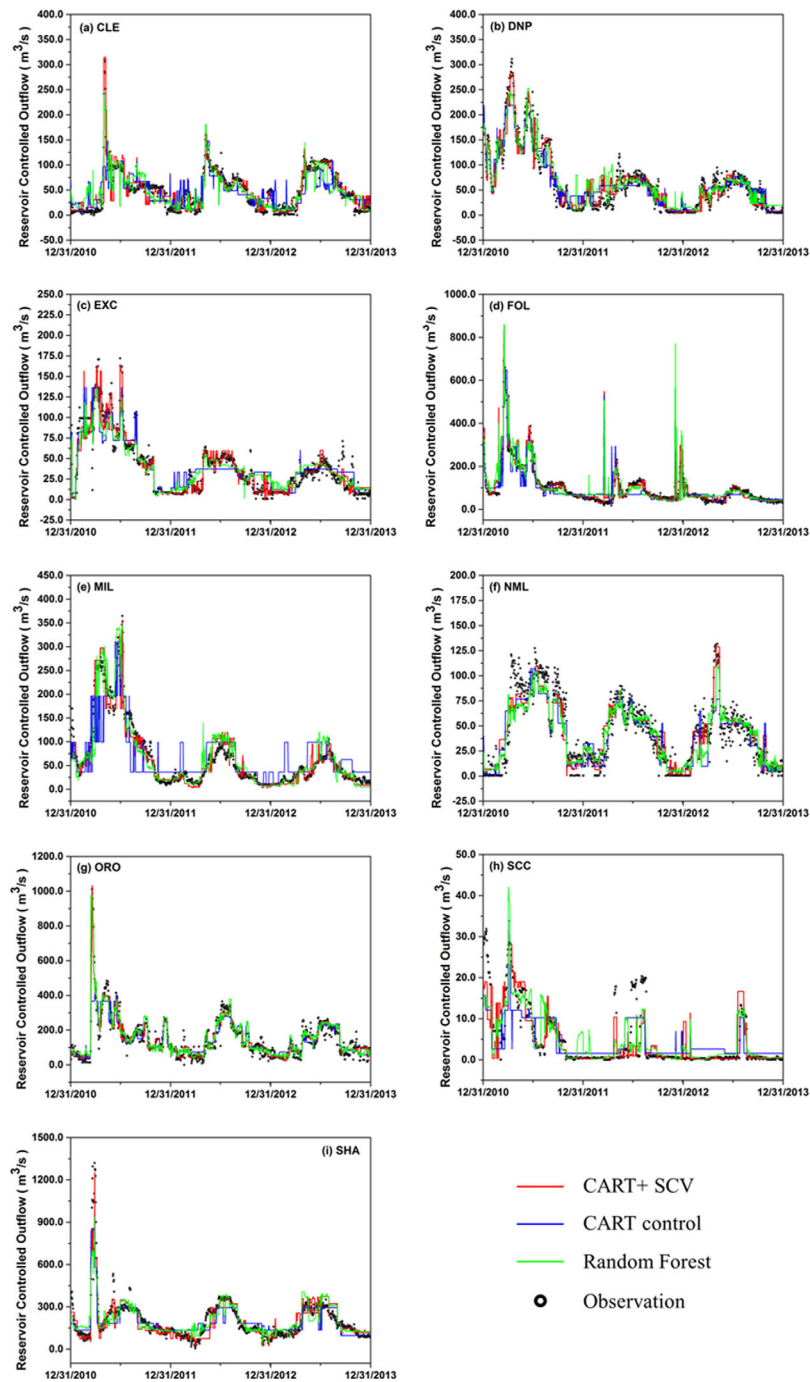
Figure 4. Reservoir controlled outflow comparison between observed daily releases (black) with the simulated releases with CART combined with shuffled cross-validation scheme (red), CART without shuffling scheme as control run (blue), and random forest (green).

$$PDIFF = Q_{obs,m} - Q_{sim,m}, \quad m = \arg\max{(Q_{obs,i})}, i \in 1, 2, \ldots, N, \tag{7}$$

where Q_{sim} and Q_{obs} are the simulated and observed outflow, respectively; $\bar{Q}_{obs}$ and $\bar{Q}_{sim}$ are the mean of the observed and simulated outflow, respectively; j is the time when maximum peak flow happens during the verification period; and N is the total number of days during the verification period.

In order to further verify the proposed model, despite of the comparison with actual releases, the storage volume changes and storage trajectories are also investigated. Using the simulated outflow and the

Table 3. Root-Mean-Square-Error (RMSE), Correlation Coefficient (R), Nash-Sutcliffe Model Efficiency (NSE), and Peak Flow Difference (PDIFF) Between the Observed Reservoir Controlled Outflow and Simulated Results With Different Methods, Including Combined CART and Shuffled Cross Validation (CART + SCV), CART With Twofold Cross Validation (CART Ctrl), and Random Forest (RF)[a]

Reservoir	Methods	RMSE (m³/s)	R	NSE	PDIFF (m³/s)
CLE	CART + SCV	**16.423**	**0.919**	**0.836**	**5.396**
	CART Ctrl	27.197	0.745	0.560	−161.452
	RF	21.447	0.850	0.720	−62.627
DNP	CART + SCV	**22.688**	**0.946**	**0.872**	**−35.762**
	CART Ctrl	23.695	0.900	0.818	−92.142
	RF	22.734	0.931	0.861	−70.624
EXC	CART + SCV	**12.034**	0.938	**0.837**	**−15.118**
	CART Ctrl	16.142	0.898	0.796	−35.426
	RF	14.622	**0.941**	0.833	−36.682
FOL	CART + SCV	**46.937**	0.901	0.701	140.299
	CART Ctrl	55.217	0.805	0.601	**−43.043**
	RF	55.081	**0.928**	0.726	167.500
MIL	CART + SCV	26.452	**0.957**	0.832	**−9.226**
	CART Ctrl	40.659	0.804	0.641	−53.703
	RF	**20.152**	0.931	**0.848**	−23.615
NML	CART + SCV	**13.913**	0.913	**0.830**	**−2.835**
	CART Ctrl	16.848	0.906	0.801	−58.618
	RF	14.707	**0.915**	0.822	−22.901
ORO	CART + SCV	**34.412**	0.960	0.920	**85.225**
	CART Ctrl	65.272	0.852	0.713	−544.229
	RF	35.793	**0.970**	**0.959**	−120.037
SCC	CART + SCV	4.734	**0.926**	**0.811**	**−12.893**
	CART Ctrl	5.688	0.897	0.735	−17.231
	RF	**4.695**	0.900	0.799	−16.789
SHA	CART + SCV	**71.466**	0.874	0.742	**−67.461**
	CART Ctrl	80.168	0.847	0.701	−964.309
	RF	74.627	**0.877**	0.748	−379.122

[a]Bold values indicate the best measure for each reservoir and each statistics.

following mass-continuity equation, we calculate the storage volume changes and storage level trajectory for each reservoir during the verification period.

$$\Delta S_t = Inflow - Outflow + Pr\,ecip. - Evapration + Gain\,\&\,Loss \tag{8}$$

$$S_t = S_{initial} + \sum_{i=1}^{t} \Delta S_t \tag{9}$$

where ΔS_t is the daily storage change at time step t; S_t is the storage volume at time step t; $S_{initial}$ is the starting storage volume.

According to equation (8), the storage daily change equals the total inputs to the reservoir subtracts the total outputs of the system. The precipitation, lake-surface evaporation, and gains and losses data are obtained from the CDEC data sets for each reservoir.
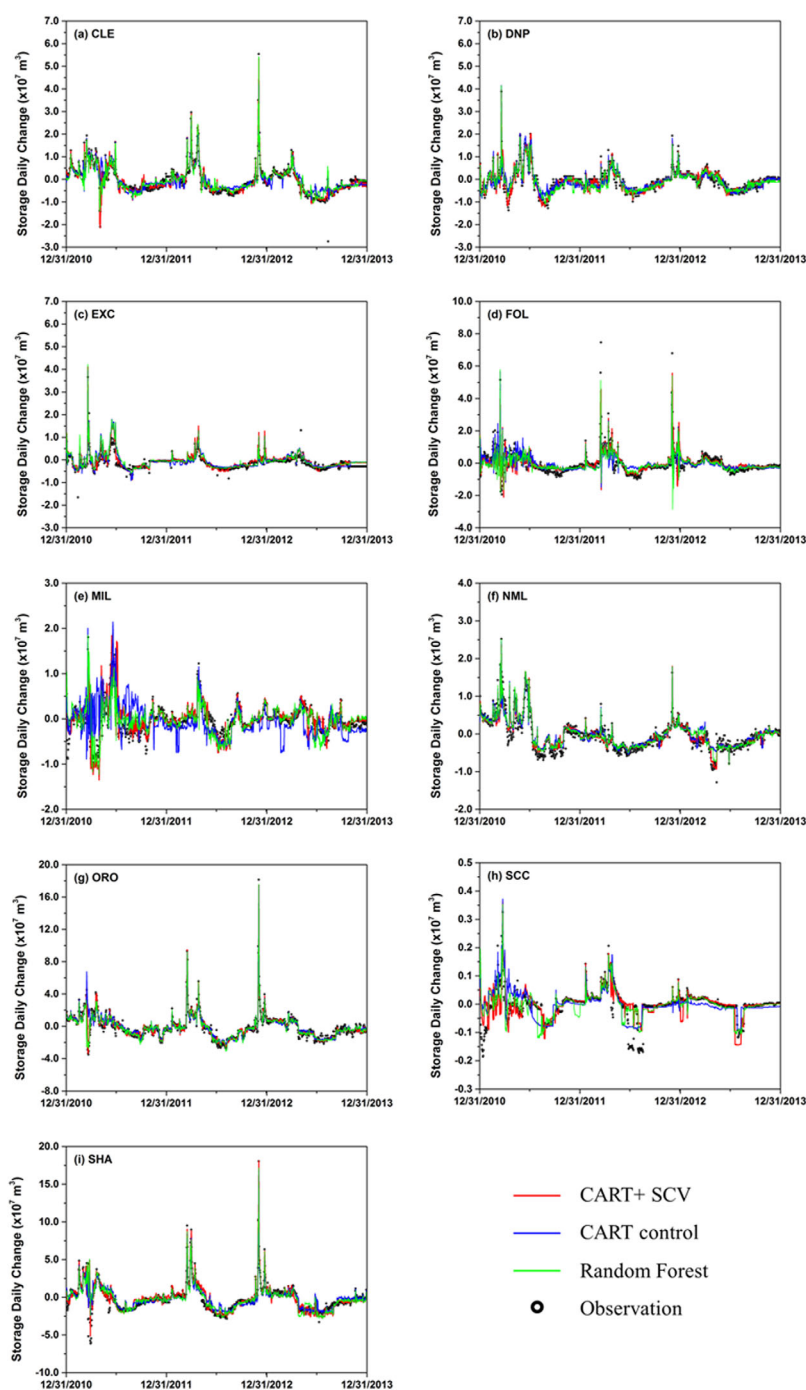
The comparison between the calculated-storage changes and the observed-storage changes is shown in Figure 5 and the corresponding Root-Mean-Square-Error (RMSE), correlation coefficient (R), and Nash-Sutcliffe Model Efficiency (NSE) are presented in Table 4.

According to equation (9), we further calculate the storage trajectories from 31 December 2010 to 31 December 2013, as shown in Figure 6. In Figure 6, the starting storage volume is fixed on 31 December 2010 for reservoirs. The storage trajectories are obtained by accumulating all the simulated daily storage changes throughout the whole verification period. The observations (black line) are the actual daily storage volume archived in CDEC. The corresponding statistics are presented in Table 5.

4.3. Importance of Decision Variables

It is of particular interest to discover which decision variable has the most influence on the reservoir operators' decisions. As we mentioned above, the Gini diversity index is used to mathematically quantify the contribution of decision variables. Generally, according to equations (2) and (3), the smaller the Gini diversity index, the purer a set of "child" node is. The Gini diversity index for a "parent" node is always higher than

Figure 5. Reservoir daily storage changes comparison between observed storage changes (black) with the calculated results with CART combined with shuffled cross-validation scheme (red), CART without shuffling scheme as control run (blue), and random forest (green).

that of two descendant nodes ("child" nodes), which indicates that the employed split using one of the decision variables is able to rationally partition the data and result in a better homogeneity in the "child." Here we first sum up the Gini diversity index of all resulting "child" nodes for all splits using each decision variable. Then, the summation of the Gini diversity index for each decision variable is normalized to a value between 0 and 1, following the rule that decision variable with smaller Gini index summation has higher normalized value. Such normalization ensures that the decision variable with higher contribution or sensitivity in generating the model output has a higher value than others. In other words, the closer the normalized Gini diversity to 1, the more efficient and dominating the decision variable is in splitting the target

Table 4. Root-Mean-Square-Error (RMSE), Correlation Coefficient (R), and Nash-Sutcliffe Model Efficiency (NSE) Between the Observed Reservoir Daily Changes and Calculated Changes Using Simulated Daily Releases[a]

| Reservoir	Methods	RMSE ($\times 10^7$ m^3)	R	NSE
CLE	CART + SCV	**0.168**	**0.959**	**0.920**
	CART Ctrl	0.254	0.907	0.817
	RF	0.209	0.937	0.877
DNP	CART + SCV	**0.162**	**0.944**	**0.885**
	CART Ctrl	0.199	0.910	0.827
	RF	0.195	0.916	0.835
EXC	CART + SCV	5.508	**0.069**	**0.083**
	CART Ctrl	**5.499**	0.043	0.067
	RF	5.504	0.056	0.055
FOL	CART + SCV	0.475	**0.800**	0.638
	CART Ctrl	0.500	0.673	0.447
	RF	**0.407**	0.782	**0.652**
MIL	CART + SCV	0.174	**0.879**	**0.730**
	CART Ctrl	0.351	0.510	0.092
	RF	**0.157**	0.858	0.727
NML	CART + SCV	**0.132**	**0.948**	0.876
	CART Ctrl	0.156	0.933	0.864
	RF	0.146	0.939	**0.882**
ORO	CART + SCV	**0.302**	**0.979**	**0.958**
	CART Ctrl	0.568	0.924	0.851
	RF	0.398	0.963	0.927
SCC	CART + SCV	**0.162**	**0.944**	**0.885**
	CART Ctrl	0.199	0.910	0.827
	RF	0.195	0.916	0.835
SHA	CART + SCV	0.664	0.932	0.854
	CART Ctrl	0.703	0.919	0.838
	RF	**0.624**	**0.937**	**0.873**

[a]Bold values indicate the best measure for each reservoir and each statistics.

variable. Using a pie-graph for each reservoir, we present the normalized decision variable importance from the CART combined with shuffled cross validation, CART control run, and random forests in Figures (7 and 8), and 9, respectively. For better illustration and discussion, the WYIs for Sacramento Valley and San Joaquin Valley in Table 2 are grouped as Dry/Wet conditions, and the six decision variables associated with river indices are categorized as runoff condition. Therefore, there are total nine categories of decision variables, which are compared in Figures 7–9, namely storage, dry/wet condition, runoff condition, SWP allocation, reservoir inflow, seasonality/month, precipitation, snow depth, and downstream river stage.

5. Discussions

5.1. Comparison of Simulated Outflows

As shown in Figure 3, the highest posterior maximum likelihood suggests that the most proper tree size in CART that allows the model has good predictive performances, and more importantly, guaranties model's stability on randomly constructed "unseen" data. The distribution shapes of the best tree depth of both CART combined with shuffled cross validation and CART control run indicate that either a larger or smaller tree might increase the prediction uncertainty. Similar experiments were presented in *Breiman et al.* [1984], in which *Breiman et al.* [1984] concluded that too small a tree will not use some of the classification information, and therefore result in a large misclassification rate. On the other hand, the misclassification rate originally decreases as tree size grows, and then climbs after it hits a minimum. For our reservoir cases, the proper tree sizes found by the CART combined with shuffled cross-validation scheme are consistently higher than that using CART only (Figure 3), because the shuffling scheme introduces more predictive information which the fixed training data set might not contain. Considering that the number of decision variable is over 10, the levels of tree selected by the posterior histogram are not too high to lose the transparency of the Boolean logic in the decision tree algorithm. Comparably, the final tree depths with random forest are significant higher than that with both CART + SCV and CART control run for each reservoir. This indicates that there are more final classes or leaves in random forest than CART algorithms than that with other two methods. In the experiments, all random forests are set to be fully grown and use the best subset of decision variable in each split instead of all variables [*Liaw and Wiener*, 2002], which is robust against overfitting [*Breiman*, 2001]. Nevertheless, this strategy in random
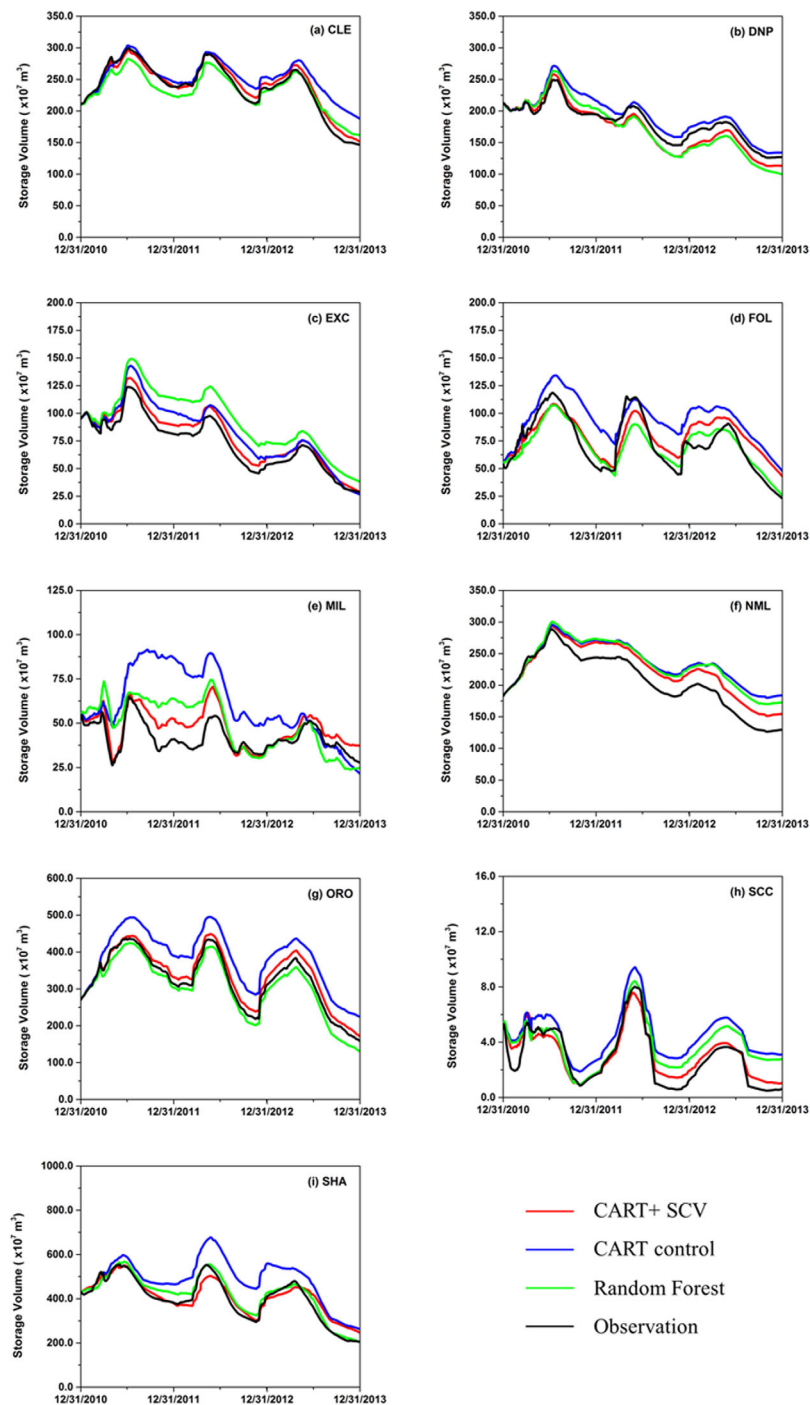
Figure 6. Reservoir storage trajectory comparison between the actual storage volume (black) with the calculated results with CART combined with shuffled cross-validation scheme (red), CART without shuffling scheme as control run (blue), and random forest (green).

forest will consequently produce a final tree with a more complex structure and a higher depth than the standard decision trees. If the tree complexity or the number of final classes is not the primary concern, then the random forest method is suggested because of its ability to provide diverse predictions. In applying the random forest method, it is also important to mention that the higher depths might result in potential loss of logical interpretation for certain splits of decision variables.

According to the comparison of simulated controlled outflows (Figure 4), in terms of the magnitude and variation, the simulated results from all scenarios (CART + SCV, CART control, and Random Forest) are very

Table 5. Root-Mean-Square-Error (RMSE), Correlation Coefficient (R), and Nash-Sutcliffe Model Efficiency (NSE) Between the Observed Reservoir Trajectories and Calculated Trajectories Using Simulated Daily Releases[a]

| Reservoir	Methods	RMSE ($\times 10^7$ m^3)	R	NSE
CLE	CART + SCV	**7.092**	**0.991**	**0.967**
	CART Ctrl	21.843	0.941	0.788
	RF	13.479	0.979	0.881
DNP	CART + SCV	**12.404**	**0.984**	**0.842**
	CART Ctrl	13.637	0.938	0.744
	RF	14.507	0.977	0.824
EXC	CART + SCV	**6.434**	**0.997**	**0.926**
	CART Ctrl	12.397	0.973	0.724
	RF	22.386	0.945	0.699
FOL	CART + SCV	14.480	0.888	0.686
	CART Ctrl	25.001	0.844	0.280
	RF	**11.183**	**0.903**	**0.784**
MIL	CART + SCV	**7.471**	**0.859**	**0.058**
	CART Ctrl	28.452	0.438	−0.052
	RF	13.583	0.630	0.015
NML	CART + SCV	**21.194**	**0.976**	**0.770**
	CART Ctrl	33.927	0.942	0.411
	RF	30.745	0.956	0.516
ORO	CART + SCV	**17.115**	0.991	0.927
	CART Ctrl	62.411	0.970	0.300
	RF	18.973	**0.996**	**0.935**
SCC	CART + SCV	**12.404**	0.978	**0.724**
	CART Ctrl	18.007	0.968	0.642
	RF	15.637	**0.984**	0.714
SHA	CART + SCV	26.889	0.969	0.887
	CART Ctrl	95.094	0.882	0.103
	RF	**24.523**	**0.973**	**0.933**

[a]Bold values indicate the best measure for each reservoir and each statistics.

similar to the observation, except the CART control run in MIL, in which numbers of stepwise predictions fail to capture the actual releases. Both of the predicted and observed releases (Figures 4b–4e and 4h) tend to decrease as the drought conditions in California become more severe after 2011. The controlled outflow peaks at the beginning of 2011 (Figures 4a, 4b, 4d, 4e, 4g, and 4i) are well predicted with the proposed method and random forest, while the CART control tends to underestimate (Figures 4d, 4e, and 4i) on almost all the cases. Notably, all methods fail to predict the first high peak in MIL and SCC (Figures 4e and 4h). In the case of SCC (Figure 4h), another following peak (around spring in 2011) is captured by all methods. However, there are some overestimates when using random forest and CART control run. Similar to the case of SCC, all methods fail to predict the first small peak in MIL (Figure 4e). Except CART control run, all other methods are able to successfully capture the second and third peak in 2011. The unsuccessful prediction on the first peak in SCC and MIL might be due to some unknown situations that current decision variables do not consider, such as an emergent water delivery request from the downstream area, the maintenance of reservoir releasing gates, special reservoir operation during drought condition [*Kelly*, 1986; *Yang et al.*, 2015], etc. The model performance could be further improved once historical records about reservoir and downstream local information are employed.

It is believed that another important factor that has critical influences on reservoir operation is the water demand. Currently, the water demand is not included in the designed decision variable set due to its availability. We think that even though the water demand from agriculture can partially be represented by storage variation and seasonality/month, the actual daily demands from residential, industrial, and agriculture are better predictors. This is because that none of selected reservoirs in the experiment are specifically built only for agriculture water-supply purposes and most of the reservoirs are associated with multiple functionalities. Nevertheless, as mentioned in the previous section, the adding of more influencing and suitable information or predictors is easy and achievable using AI&DM techniques.

The statistical performances of the simulated outflows are satisfactory for all methods. Generally, the NSEs of each reservoir range from 0.560 to 0.959 (Table 3). According to *Moriasi et al.* [2007], model simulation can be judged as satisfactory if NSE is greater than 0.50 for streamflow. According to Table 3, some reservoirs are easier to simulated (has higher NSE values) than others. Even though the selected reservoirs have different locations, sizes, and watersheds characteristics, we think that the difficulties in simulating the
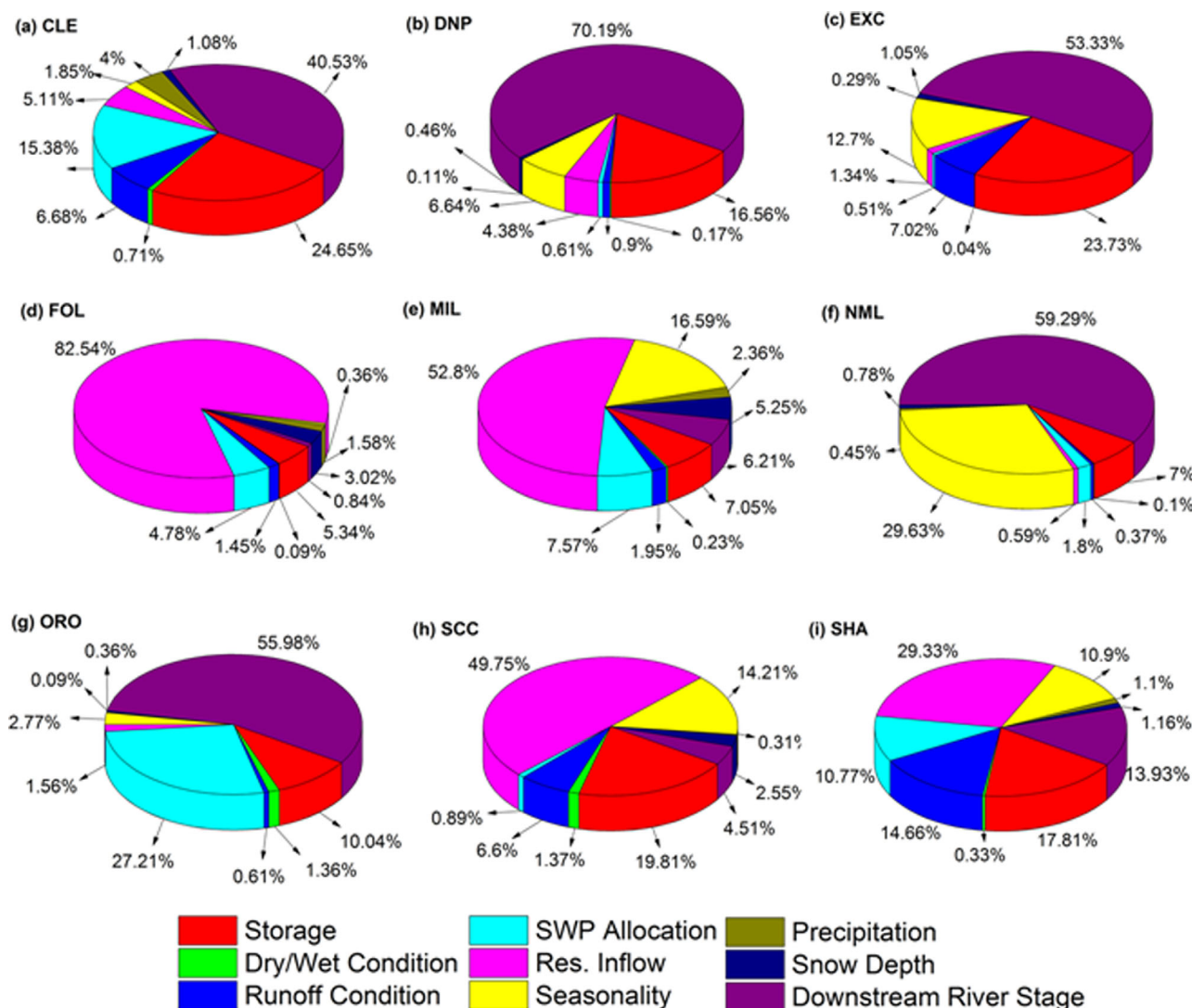
Figure 7. The normalized Gini diversity index or the importance for each decision variable for each reservoir with CART combined with shuffled cross-validation scheme.

releases are largely due to the reservoir's functionalities and the predictivity of the decision variables. Most of the selected reservoirs are located along the Sierra Nevada Mountain (Figure 1) and the snowmelt during runoff season is the main supplement for reservoir inflow, the local hydrology's influences on the operation complexity could be negligible.

As shown in Table 3, CART combined with shuffled cross-validation scheme outperforms the other two methods for four out of nine reservoirs with regard to RMSE and NSE values, while the results for the other five reservoirs are very competitive to the best values generated by either random forest or CART control run. For each reservoir, the RMSE, correlation coefficient, and NSE values with CART with shuffled cross vali-dation and random forest are higher than CART control run, which indicate that these two methods have superior performances over the original CART algorithm in our study cases. Except for FOL, the Peak Flow Difference (PDIFF) calculated with CART combined with shuffled cross-validation scheme is consistently smaller than that with the other two methods. Even though the CART control run can reach smaller Peak Flow Difference value for FOL, the calculated RMSE, R, and NSE are all worse than that with the other two methods. Comparing CART control run with random forest, the latter seems to have better performances on predicting the peak flows, especially for SHA (Shasta Lake) and ORO (Oroville Lake), and random forest has consistent higher correlation coefficient values. In daily reservoir operation, the response to peak flow is always of great importance. When there is a high flow, effective and efficient operation considers the resil-ience of reservoir so that proper amount of water is stored for future sustainable supply. More importantly,
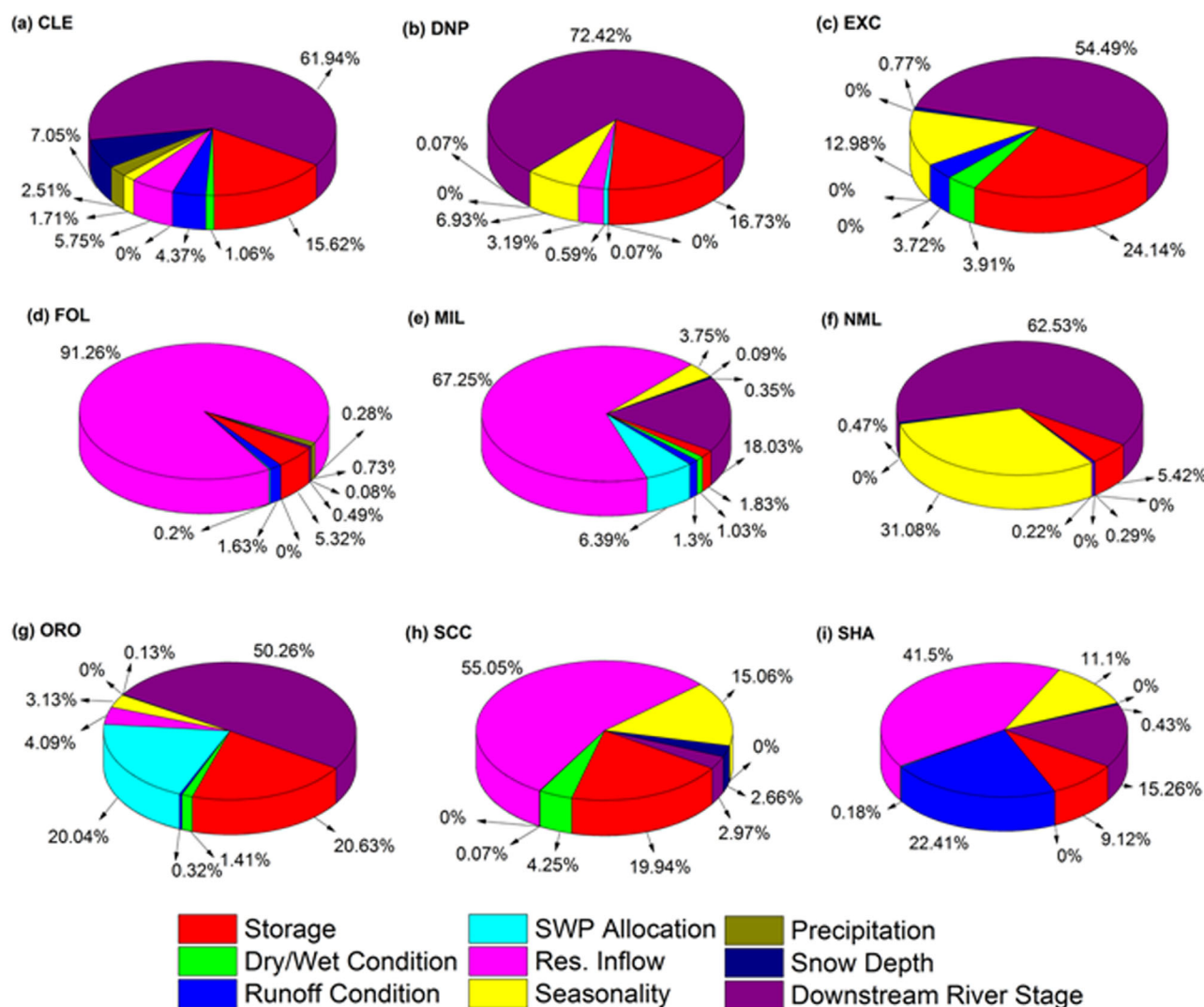
Figure 8. The normalized Gini diversity index or the importance for each decision variable for each reservoir with CART combined with CART control run.

an actual release decision needs to prevent the downstream area from flooding even an increase of release or a deliberate spill is needed. This is also the reason that downstream river stage information from each reservoir's service area is included as one of the model inputs. With respect to the overall performances on RMSE, R, NSE, and PDIFF, CART combined with shuffled cross-validation scheme will be able to more effectively predict the expert reservoir release decisions than the other two methods, especially under peak flow conditions.

5.2. Comparison of Storage Daily Changes and Trajectories

In Figures 5 and 6, the storage daily changes and storage trajectories are presented and the corresponding statistics tables are shown in Tables 4 and 5, respectively. In Figure 5, the calculated storage daily changes from all methods are very close to the observed values, especially for CLE, DNP, EXC, MNL, ORO, and SHA (Figures 5–5c, 5f, 5g, and 5i). The major discrepancies between the simulated values and observation happen in predicting three positive peak changes in FOL, two negative changes in SCC (Figures 5d and 5h), and some midlevel changes in MIL (Figure 5e). The differences are mainly due to the discrepancies between observed and simulated releases (Figure 4), as well as the errors in quantifying the losses and gains in each reservoir, such as the overestimates on reservoir evaporation, and unmeasured tributary inflows to reservoirs, which tend to cause positive changes in daily storage. Comparing the RMSE, R, and NSE values in Table 4, CART with shuffled cross-validation scheme overperforms other two methods in CLE, DNP, ORO,
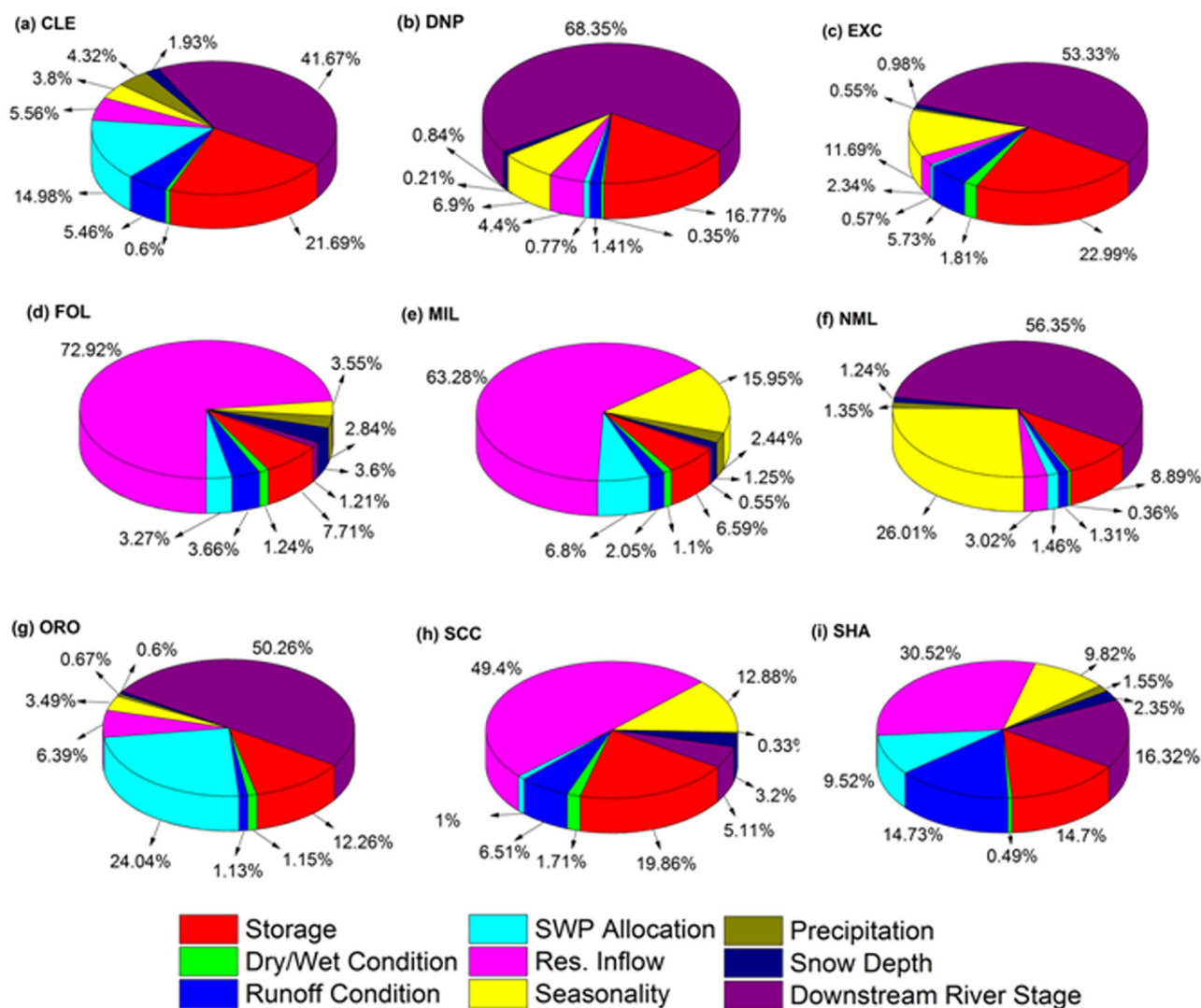
Figure 9. The normalized Gini diversity index or the importance for each decision variable for each reservoir with CART combined with random forest.

and SCC, while random forest is superior over other two in SHA. With regard to other reservoirs, the statistic values with CART with shuffled cross-validation scheme and random forest are competitive and slightly better than the CART control run.

Using the storage daily changes, the storage trajectories are further calculated with a forced starting value (on 31 December 2010) for reservoirs. Figure 6 shows the comparison between the calculated storage trajectories and observed storage volume. The corresponding RMSE, R, and NSE values are shown in Table 5. As shown in Figure 6 and Table 5, CART control run seems to give the worst simulation results of storage trajectory, and the differences to observation are relatively larger than the other two methods, especially for FOL, MIL, ORO, SCC, and SHA (Figures 6d, 6e, and 6g–6i). Random forest is able to give better results than the CART control run and the simulation results are similar to that with CART combined with cross-validation scheme in CLE, DNP, FOL, ORO, and SHA (Figures 6a, 6b, 6d, 6g, and 6i). In some cases, such as EXC, MIL, NML, and SCC (Figures 6c, 6e, 6f, and 6h), the simulation results with CART combined with shuffled cross validation are slightly better than that with random forest. According to the statistics presented in Table 5, CART with shuffled cross-validation scheme is able to produce better RMSE, R, and NSE in five out of nine reservoirs, including CLE, DNP, EXC, MIL, NML, and SCC. Random forest overperforms the other two methods in FOL and SHA. For CART control run, a dramatic discrepancy in matching actual storage trajectories is observed in MIL. The primary reason is the failure of predicting the magnitude and variations of

discharges during 2011. The differences between simulated and observed daily releases accumulate over time and result relatively large discrepancy in storage trajectories. Generally, the results produced by CART with shuffled cross-validation scheme can reach the best statistics for most of the study cases as compared to other methods, and the calculated storage trajectories using the proposed method are significantly closer to observation than the CART control run.

Due to the fact that the storage trajectory is calculated by accumulating the daily storage changes to the starting storage volume, errors in certain days might be cancelled with each other. For example, an overestimate on the first day and an underestimate on the second day might induce a near-perfect storage volume on the third day. Another potential uncertainty source is the autoregulation characteristics of the model. A fully regulated or perfectly trained model would produce a storage trajectory that repeatedly crosses the actual storage trajectory, such as only limited periods shown in the CLE, FOL, SCC, and SHA cases (Figures 6a, 6d, 6h, and 6i). In an ideal case, a given model may predict a low release once the storage volume is low and a high release when the storage volume is high. Such a model could regulate the simulated storage volume to remain within an acceptable uncertainty range. However, the autoregulation effect could be weakened by different model settings. In our designed experiment, the temporal resolution is daily and storage volume is only 1 of the 15 variables. Therefore, the model's autoregulation capacity is limited. For example, model might find out daily inflow to be more strongly correlated with daily release decisions than the storage volume. This is because the actual release contains relatively high noise while storage variations are always slower and smoother.

Even though the two facts mentioned above might result in errors and uncertainties in storage trajectories, a robust storage trajectory calculation employed in this study is still able to give decision makers certain confidence in evaluating the model performances, especially for seasonal time scale or shorter prediction lead time. As the confidence in the quality of input data deteriorates, shorter prediction or simulation time scales will become more realistic and operational, such as seasonal scale or weekly scale. Shorter time scale simulation will allow users to recursively test model performances and gradually adjust model settings and forcing data. Longer period of simulation will inevitably bring more uncertainty in the results and cause hesitations from decision makers to practically use the AI&DM techniques. Nevertheless, the validation and test should be conducted in relatively long time scale, such as years, to expose both pros and cons of any proposed simulation model.

5.3. Reservoir Operation Patterns

As mentioned in section 3.4, the decision variables contributions are measured by the normalized Gini diversity index, which allows a sensitivity analysis of the decision variables and discoveries of certain reservoir release patterns. According to Figures 7–9, one interesting finding is that without any prior information, all methods consistently detect that the historical release decisions in the Oroville Lake are very sensitive to the changes of SWP allocation. On average, the SWP allocation explains over 24% of the total variations of ORO's releases decisions according to Figures 7–9. As the most vital fresh headwater supply source for the SWP delivery, the Oroville Lake provides about 4.317×10^9 m^3 of water every year to 29 state water agencies in the central and southern parts of California. The SWP water delivery obligation makes the Oroville Lake very unique among all the nine reservoirs. The contribution percentage of SWP allocation amount ranks as the second largest one among all decision variables and the decision variable with the largest contribution is the downstream river stage.

Different from the consistent model results in ORO, both CART combined with shuffled cross validation and random forests find out that the contributions of SWP allocation are about 10% and 15% in explaining the historical release patterns in the Shasta Lake (Figures 7i and 9i) and Trinity Lake (Figures 7a and 9a), respectively. Comparably, CART control run shows there is nearly 0% contribution from SWP allocation (Figures 8a and 8i). The Shasta Lake and the Trinity Lake (CLE) are the largest and second largest reservoirs, respectively, in the California's Central Valley Project (CVP). Part of the SHA and CLE releases will flow to the Sacramento River and merge with the water from the Feather River. Eventually, the merged streamflow is jointly used and delivered to the Central and Southern California for agriculture, residential, and ecological uses, according to the multiagencies water sharing agreements between SWP and CVP [*DWR*, 2005, 2009, 2013b; *USBR*, 2004]. Therefore, it is reasonable to infer that the SWP allocation can also impact the reservoir operation decisions in both Shasta Lake and Trinity Lake. The contributions of SWP allocation could be limited in these

two reservoirs as compared to the main headwater source of SWP, which is Oroville Lake. According to Figures 7 and 9, the contributions of SWP allocation on the release decisions in SHA and CLE are estimated to be 10–15% lower than that in the Oroville Lake. The fact that CART control run fails to detect the influence from this variable in SHA and CLE is mainly due to that the best tree depth of CART control run reaches maximum values around 9 and 7 for CLE and SHA, respectively. The final tree depth with CART control run is consistently smaller than that with other two methods (Figure 3). The trees developed by CART control run might not be fully grown or even not using the SWP allocation variable in splitting the training data.

Another interesting finding is that the reservoir inflows play a more important role in the reservoirs with lower elevations. According to Figures 7–9, the contributions of inflows account for over 50% of the total variation of the release decisions in FOL and MIL, which is in agreement among all methods. Surprisingly, FOL and MIL are the two reservoirs with the lowest elevations as compared to others. The elevations of FOL and MIL are 142 and 177 m, respectively (Table 1). It is believed that for the low-elevation reservoirs, the operation rules turn to be more simplistic when it is compared to those in high/medium elevation reservoirs. With less risk of being suffering from flooding, the priority of water supply for low reservoirs becomes higher. Moreover, low-elevation reservoirs have fewer obligations to transfer water to other areas, because they are already closer to water demand areas, such as farmland, residents, and industry, as compared with high/medium elevation reservoirs. The operation rules for these reservoirs are mostly to mitigate the deficiency between the available water and demands. In other words, the management of the outflows depends mostly on the available water that these reservoirs receive from upper-stream area, which is the inflow amount. Despite of the agreement that all methods detect inflow is the most important variable in explaining releases in FOL and MIL, the inflow contribution estimations with CART control run are relatively higher than that with the other two methods. In the case of MIL (Figure 8e), the CART control run quantifies that the influence from seasonality on release decisions is about 3.75%, which is significantly smaller than the estimates from CART with shuffled cross validation (Figure 7e) and random forests (Figure 9e). Because the Firant Dam (MIL) is located in the central valley area of California (Figure 1), where agriculture activities and farm lands are intensive, the seasonal demands for irrigating crops can significantly impact MIL's release decisions. Even though the CART control run underestimates the influences from seasonality, the contribution from downstream river stage is found to be significantly larger than that with other two methods. It is possible that the seasonality changes are also embedded in the variation of downstream river stage. The dependence among decision variables will be further discussed in the next section.

With regard to the low-elevation reservoirs, we further investigate the extreme case of the Folsom Lake, in which models show that the inflow is largely dominating over 80% of the reservoir release decisions. We find out that the spill events in Folsom Lake are more frequent and intensive than other reservoirs. During the spill events, most of the rule curves designed for flood control, water supply, or hydropower generation will be no longer applicable, and the inflow and outflow are almost equivalent to each other, which results in a high correlation between inflow and outflow. However, the high dependence between these two variables does not undermine the argument that sometimes the storage-release rule curve has its limitation and might not sufficiently represent the actual release decisions. We think that the use of AI&DM techniques, which directly fits the actual releases with multiple decision variables, is able to rationally mimic the historical expert reservoir operation and provide transparent and logical representation of daily decision making process.

According to the Figures 7–9, it is also noticed that the operation of many reservoirs rely on the downstream river stage. We infer that it is because the downstream status is very crucial to release operation during high flow periods. Traditional flood control rules are highly dependent on seasonality and may have different rule curves for various months. However, if the downstream river status already exceeds a certain level and the reservoir storage-based rule curves still allow extra releases, the reservoir operator has to intentionally reduce the releases, therefore, deviate from the predefined graphical operating policies/rules. We also expect that there are other similar situations that the actual releases are different from a predefined rule curve, such as when an urgent water delivery requests are made by downstream users, or a change of SWP allocation, or a facility suddenly temporarily becomes off-line.

Also, we carried out a sensitivity test of removing downstream gauge information from the experiments. We found out that the contribution of seasonality/month dramatically increased for the Oroville Lake (ORO), New Melones Reservoir (NML), and Trinity Lake (CLE), which indicated that the downstream river stage

could have a dependence on seasonality. However, for other reservoirs, such as EXC, DNP and MIL, after removing the downstream gauge information, the contribution from seasonality/month decreased. It means that both downstream river stage and seasonality are two important variables for operating these reservoirs in general. Using the proposed scheme, various sensitivity analyses could be carried out to test a specific predictor's contribution, as well as the general reservoir operation patterns.

Similar to the downstream river stage, reservoir storage volume is also found to be an important decision variable by all methods. In California, the operation of reservoirs is all guided by USACE, which primarily uses empirical rule curves to regulate releases for flood control purposes. The rule curve is basically a graphical representation of the relationship between releases amount and storage volume or water level. All methods are able to identify that the storage volume has significant impacts on the reservoir releases, except for the case of CART control run in MIL (Figure 8e). According to the results from CART with shuffled cross validation (Figure 7) and random forest (Figure 9), the influence of storage volume on release decisions for the nine major reservoirs varies from 5% to 24%. This finding is also in agreement with *Giuliani et al.* [2015], in which the reservoir storage is automatically detected by a proposed Information Selection and Assessment (ISA) framework as one of the most important variables in improving the operating policy in the Hoa Binh reservoir in Vietnam. In *Giuliani et al.* [2015], besides the storage volume, other sensitive decision variables are streamflow and time. In our case, there are three types of model inputs (inflow, downstream river stage, and seasonality) are found to be important with respect to the reservoir operations in California.

Nevertheless, as compared with other decision variables, such as downstream river stage or inflow, reservoir storage has less influence on daily release decisions as shown in Figures 7–9. We believe there are several reasons. First, the experiments are conducted in a daily temporal scale. Therefore, the controlled releases contain many high-frequency variations as it is shown in Figure 4. Given a similar noise pattern in other decision variables, such as inflow or downstream river stage, regression models tend to underestimate the contribution of storage volume, which always exhibit relatively smooth variations with seasonal and periodic patterns (Figure 6). Another reason is that under certain circumstances, such as continues drought conditions or sudden change of water supply and demand, the daily release decisions can deviate from the USACE release guidance and the rule curves, of which the primary purpose is to reduce the risks of seasonal floods and prevent the reservoir from draining. Last but not least, the dependence between the historical storage volumes and the seasonality, which is another model input, can be strong enough so that the regression models mistakenly overestimate the contribution from seasonality and underestimate the actual contribution of the storage-based operation. The influence of storage on release decisions can be embedded into the seasonality impacts, especially when a relatively large seasonality contribution is observed, such as the cases of EXC, MIL, NML, SCC, and SHA from Figures 7 and 9.

Due to many security issues, the actual rule curves in California are not public accessible, which prevents us from further investigating whether the proposed model can accurately estimate the influences of storage on release decisions. A comparison between the artificially generated release with the one that strictly governed by USACE operating manuals will allow a more insightful understanding on reservoir operation in practice, as well as a great support in improving the current reservoir simulation models. Nevertheless, the proposed model could also be used in parallel with the operating rule curves to give more confident guidance on reservoir releases, because the presented regression models not only rely on storage, but also include many other decision variables, which are not graphically drawn in the storage governed rule curves.

5.4. Limitations and Further Improvement
One of the limitations of this study lies in the assumption that decision variables are not significantly dependent to each other, which might not be always be true. For example, storage volume, precipitation, downstream gauge, and snow depth might be correlated to seasonality/months. From the model developer point of view, in an ideal case, the selected model inputs are supposed to be strictly independent to each other. However, due to the nonlinearities brought by coupling of natural process and complexity in human decision making process, to reach the ideal case is extremely hard. The current 15 types of model inputs are selected based on the availability of data, the consultations and suggestions from USACE reservoir operators, CDWR hydrologists, local decision makers, and anonymous reviewers. In reality, the information required for making a practical release decision varies from one reservoir to another, as well as from one

specific region to another. Nevertheless, the current model inputs include most of the important information in reservoir operation in California. Users are recommended to employ customized model inputs for their regions of interests and modify model settings. With regard to removing the dependence among decision variables, a principal component analysis could be further employed to transform decision variables into orthogonal coordinate system. However, the physical interpretation of variables will be compromised.

A further improvement of prediction accuracy involves the consideration of reservoir's connectivity. In some cases, one reservoir's outflow becomes a lower reservoir's inflow when reservoirs are physically in series, such as a cascade reservoir system. The study of cascade reservoir system is excluded in this study and all the selected reservoirs are belonging to different river basin. However, it is achievable to set the outflows and operation rules from/of an upper reservoir as the model inputs for a lower reservoir using the same approach demonstrated in this paper. By properly connecting the inputs and outputs of two independent models, the intrusion of reservoir-connectivity could be further investigated and analyzed.

In California, another nonphysical aspect that influences the daily releases is the systematical and large-scale operation on certain reservoirs controlled by the same agency. For example, in some circumstances, USBR operates its reservoirs in a systematical manner, in which certain patterns of increasing or reducing releases can happen to all USBR controlled reservoirs at the same time. Such kind of state-wide operation is absent from current experiment, which needs to be further addressed by designing proper conceptual indicators or decision variables. To design such variable requires a mathematically quantification of an operating agency's behavior. In this paper, a similar variable is the SWP allocation, which quantifies the water delivery operation from the CDWR. With regard to the physical connectivity issue and the influences from large-scale operation, the reservoirs in this study are carefully chosen. Our selected nine major reservoirs are not physically connected. In other words, the selected reservoirs belong to different river basins (Table 1). Moreover, the reservoirs involved are operated by different agencies so that the influence from a large-scale operation can be reduced.

Future works are suggested to focus on the following aspects that currently not included in this study. As mentioned above, a comparison with an actual reservoir rule curve is needed to further evaluate the inter-operation of the artificially generated releases. Another focus will be on investigating the impacts of water quality requirements, ecosystem water demands, and economic costs of water and electricity on reservoir water supply or hydropower release decisions. Currently, authors are unable to define a suitable indicator or mathematical quantification of the impacts from environment and ecosystem as additional model inputs. Last, it will be interesting to combine the regression techniques with optimization algorithm with the purpose of deriving optimal and rational releases for specific operation objectives, such as minimizing water shortage and flood risks, maximizing hydropower generation and efficiencies for irrigation and water supply, etc. Even though the mathematical definition of objective functions might be subjective, which obstructs the closing of the gap between theoretical and realistic, the predicted outflows from this study can be used as an initial solution and baseline that represents the expert reservoir release decisions.

6. Conclusion

In this paper, a simple, transparent, and efficient decision tree model is proposed to simulate the controlled outflows from nine major reservoirs in California. The inputs of the predictive model include storage, precipitation, reservoir inflows, SWP allocation amounts, wet/dry conditions, runoff conditions, snow depth, and downstream river stage information. These decision variables are becoming significantly crucial to understand and predict human's behavior on reservoir release operations. The results with proposed approaches are compared with original CART with twofold cross validation, random forest, as well as observations during the verification period. A decision variable sensitivity study is carried out using the Gini Diversity index and the results with different methods are compared. In general, this study provides a novel application of using AI&DM techniques, primarily decision tree methods, on reconstructing and predicting the daily expert reservoir release decisions based on historical records.

In respect to the employed methodologies, the following conclusion can be drawn:

1. Studies on nine major reservoirs in California show that the CART combined with shuffled cross-validation scheme and random forests are superior over the CART control run.

2. The proposed shuffled cross-validation scheme, which is intended to break the structure of training data set and recursively calibrate the decision tree depths, is able to enhance the regression accuracy of CART as shown based on an independent verification data set using RMSE, correlation coefficient, NSE, and Peak Flow Differences as measures.

3. The CART combined with shuffled cross-validation scheme has slightly better performance over random forests on simulating peak releases, which are crucial for downstream flood control.

One drawback of using the enhanced CART algorithm could be the lack of smoothness of prediction due to the selected final tree depths. It is observed that the final tree depth selected by the enhanced CART algorithm is smaller than that with random forests. Random forest is recommended if users prefer a larger number of final classes and a relatively smoother prediction. Furthermore, because the shuffled cross-validation scheme recursively examines the posterior performances with multiple CART runs in the training phase, the computation time is higher than other two methods. However, once model finishes its training, all of the methods are efficient for predicting release decisions and the runtimes are similar to each other based on our experience using the same validation data set.

The use of decision tree methods on nine major reservoirs in California also provides us with some findings for the current reservoir operation in California:

1. Without any prior information, CART combined with shuffled cross validation and random forests find out that the Oroville Lake (ORO), Trinity Lake (CLE), and Shasta Lake (SHA) are the three reservoirs intensively dominated by the changes of SWP allocation; the SWP allocation can explain about 20%–27% of the variations of release decisions in Oroville Lake. Because the Oroville Lake is the largest headwater reservoir for the California's SWP, the influence of SWP allocation amount is automatically detected and quantified to be the largest as compared to other reservoirs.

2. Three methods are in agreement with the fact that low-elevation reservoirs, such as the Folsom Lake (FOL) and New Melones Reservoir (NML), are operated under considerably large influences from the inflow amounts, which is mainly due to their closeness to demand areas and spill events effects.

3. In general, reservoir storage volume, seasonality, and downstream river stage are extremely important variables for operating the reservoirs in California. These variables are representing USACE's operating rule curves for preventing floods and maintaining water supplies. For the nine reservoirs involved in this study, the contributions of decision variables vary from one reservoir to another, because the sizes, main functionalities, and operating rules can be different.

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