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Improving the accuracy of K-nearest neighbour method in long-lead hydrological forecasting

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Abstract. The nonparametric regression method of K-Nearest Neighbour (K-NN) has **KEYWORDS** been used in a variety of eco-hydrological issues. In this study, some techniques were K-NN; presented to improve the accuracy of the K-NN method in forecasting accumulated 9-Hydrological month inflow, from 1971 to 2001, of Zayandeh-rud dam in Iran, from winter to the end of the forecasting; following summer. The considered improving techniques consisted of: 1) selecting the best HBMO: data preprocessing functions, 2) selecting the best number of neighbours, 3) selecting the Zayandeh-rud; best distance functions, 4) specifying the best weights of predictors at distance functions, Iran. and 5) adding the ability of extrapolation to K-NN using a proposed method. Final results showed that the use of the mentioned techniques had promoted the accuracy of K-NN's forecast, meaningfully. The results of goodness-of-fit criteria for the optimized K-NN in comparison with a regular K-NN presented an increase by 31% in correlation coefficient (from 65% to 96%), a decrease from 31% to 8% in volume error, and finally a drop from 54% to 25% in the root mean square error. © 2016 Sharif University of Technology. All rights reserved.

1. Introduction

Data-driven methods are powerful means to be used in different issues such as pattern recognition, categorizing, estimating, and forecasting. These methods can be divided into two main groups of parametric and nonparametric models, in which K-Nearest Neighbour (K-NN) method is one of the most acknowledged nonparametric ones [1]. In the past decades, K-NN has been applied in a variety of areas such as density estimation [1], rainfall-runoff forecasting [2], resampling hydrologic time series [3], generating regional climate scenarios [4], short-term traffic flow prediction [5], wind power forecasting [6], short-term rainfall predictions [7], probabilistic streamflow fore-

*. Corresponding author. Tel.: +613 9905 4957; Fax: +613 990 54944 E-mail addresses: mohammad.azmi@monash.edu (M. Azmi); fahimeh.sarmadi@monash.edu (F. Sarmadi) casts [8], modelling hydrological time series [9], shortterm foreign exchange forecast [10], and long-term rainfall probabilistic predictions [11].

Regarding long-lead hydrological forecast by K-NN, Araghinejad and Burn [12] showed that the use of a combination of K-NN and geostatistical methods in hydrological forecasting can lead to more reliable results in long-term management of water resources. Further, Asadiani Yekta [13] presented that a combination of K-NN algorithm and ANFIS model could be successfully applied in estimating inflow suspended load to dams. Later, Azmi et al. [14] proposed a K-NN based data fusion method for short-term and long-term hydrological forecasting.

Generally, some advantages of K-NN method in forecasting and estimating issues are simplicity, no calibration stage, modelling the nonlinear processes, and ability to cope with numerous predictors [9,15]. However, there are limitations such as requiring enough historical time series to recognize similar events and inability at extrapolating output, which need to be addressed appropriately [8,9].

2. General algorithm of K-NN in hydrological forecasting

The concept of K-NN method is based on observing values of the predictor variables in the current time and then searching for similar conditions amongst historical events. These similar conditions can be considered as possible solutions depending on the degree of similarity. In this method, Kernel function is used as a nonparametric distribution function. The general algorithm of K-NN is as follows:

- 1. Preprocessing values of all predictor variables;
- 2. Setting a matrix with m columns (the number of predictors) and n + 1 rows (the length of time series);
- 3. Assuming the last row of the above matrix as a vector of predictors at the current time $(x_{j,t}, j = 1 : m)$;
- 4. Assuming the remaining rows as a matrix of predictors at historical time series $(x_{j,t-i}, j = 1 : m, i = 1 : n);$
- 5. Defining the vector Q with n rows of independent variable values from t n to t 1;
- 6. Using distance function, distances between $x_{j,t}$ and $x_{j,(t-i)}$ are calculated as:

$$Dist(t-i) = f(w_j, x_{j,(t-i)}, x_{jt}),$$
(1)

where, w_i is the weight of predictor variable j;

- Sorting distances vector (Dist) from minimum to maximum (SDist) and correspondingly sorting vector Q based on SDist;
- Selecting the best number of neighbours (k) based on some methods which will be explained in Section 3.3;
- 9. Applying a discrete Kernel function [1] to give weights to k neighbours as follows:

$$S(e) = \frac{1/S\text{Dist}(t-e)}{\sum_{e=1}^{k} 1/S\text{Dist}(t-e)} \quad e = 1...k$$
(2)

10. Forecasting the values as follows:

$$Forecast = S \times Q^T, \tag{3}$$

where, T is the transpose operation.

3. The best selection of effective components at K-NN

The main components of K-NN include data preprocessing functions, distance functions, weights of predictors at distance functions, the number of neighbours, and extrapolation stage.

3.1. Data preprocessing functions

It is necessary to make the range of all variables consistent. The following functions are commonly used in data preprocessing [16]:

1. Auto scaling:

$$X_{ij} = \frac{x_{ij-m_j}}{\sigma_j},\tag{4}$$

where, x_{ij} is the value of predictor j at time i; m_j and σ_j are the average and standard deviation of predictor j at historical time series, respectively;

2. Range scaling:

$$X_{ij} = \frac{x_{ij} - L_j}{U_j - L_j},\tag{5}$$

where, L_j and U_j are the minimum and maximum values of variable j at historical time series, respectively;

3. Maximum scaling:

$$X_{ij} = \frac{x_{ij}}{U_j}.$$
(6)

4. Profiles:

$$X_{ij} = \frac{x_{ij}}{\sqrt{\sum_{i=1}^{n} x_{ij}^2 \sum_{j=1}^{m} x_{ij}^2}}.$$
 (7)

5. Principal Component Analysis (PCA). This method has been used in a variety of applications to reduce the volume of information and number of variables contributing to a model [17]. In fact, after performing PCA on predictor variables, the aggregated variables are considered as new predictor variables.

3.2. Distance functions

The following distance functions are commonly used in K-NN method. In the following distance functions, x_{ij} is the value of predictor j at time i, and w_j is the weight of predictor j:

1. Euclidean distance function:

$$Dist(t-i) = \sqrt{\sum_{j=1}^{m} w_j \left(x_{j,(t-i)} - x_{j,t} \right)^2}.$$
 (8)

2. Manhattan distance function [18]:

$$Dist(t-i) = \sum_{j=1}^{m} w_j |x_{j,t} - x_{j,(t-i)}|.$$
(9)

3. Mahalanobis distance function [19,20]:

$$Dist(t-i) = \sqrt{(x_t - x_{t-i})^T C^{-1} (x_t - x_{t-i})},$$
(10)

where, C^{-1} is the inverse of covariance matrix.

4. Camberra distance function [18]:

$$\text{Dist}(t-i) = \sum_{j=1}^{m} w_j \left(\frac{x_{j,t} - x_{j,(t-i)}}{x_{j,t} + x_{j,(t-i)}} \right)^2.$$
(11)

5. Lance-Villiams distance function [18]:

$$\operatorname{Dist}(t-i) = \frac{\sum_{j=1}^{m} w_j \left| x_{j,t} - x_{j,(t-i)} \right|}{\sum_{j=1}^{m} w_j \left| x_{j,t} + x_{j,(t-i)} \right|}.$$
 (12)

6. Cosine Coefficient function [21]:

$$\text{Dist}(t-i) = \frac{1}{m} \left(\sum_{j=1}^{m} w_j \frac{x_{j,t} \times x_{j,(t-i)}}{x_{j,(t-i)}^2} \right), \quad (13)$$

where, m is the total number of predictor variables.

3.3. Selecting the number of neighbours and specifying weights at distance functions

Three common methods to determine the number of neighbours are:

- 1. Personal experiences (Empirical methods): Different researchers have tried to find explicit equations to estimate the best number of neighbours and weights of predictor variables at distance functions. Here, the equation $K = \sqrt{n}$ is used as an approximation of the best number of neighbours [22]. In this equation, n is the length of historical time series and K is the approximated number of neighbours in K-NN method. The performance of this equation improves with increase in the length of time series. Further, weights of predictor variables at distance functions can be specified by user subject to professional experiences;
- 2. Trial and error methods: This method tries to determine the best number of neighbours and weights of predictor variables at distance functions by following a trial and error process. Generalized Cross-Validation (GCV) defined by Tarboton et al. [22] is presented as follows:

$$GCV = \frac{\sum_{i=1}^{n} \operatorname{err}_{i}^{2} / n}{\left(1 - 1 / \sum_{l=1}^{k} 1 / l\right)^{2}},$$
(14)

where, n is the total number of samples (here, time spans), err_i is the forecasts errors at time i, and k is the best number of neighbours. Here, number of neighbours and weights of predictor variables, which lead to minimum value of GCV, are considered as the optimum solution. The main problem of this method is to determine the space of solutions as well as being highly time consuming, which can be persuasive to consider evolutionary optimization methods; 3. Evolutionary optimization algorithms: Evolutionary optimization methods are indeed the advanced form of the previous technique (trial and error process). In the current research, Honey-Bee Mating Optimization (HBMO) algorithm was applied to derive the optimum values of number of neighbours and weights of predictors at distance functions via minimizing the values of GCV (Eq. (14)). Over the past decade, HBMO has been used in different environmental subjects [23,24]. More information about the procedure and state-of-art of HBMO algorithm can be found at Sabbaghpour et al. [25].

3.4. Extrapolation in K-NN method

In order to overcome the limitation of K-NN method in extrapolating the forecasts, the following method is proposed:

1. Deriving errors of forecasts of the training stage:

$$E = [Z_i] - \lfloor \hat{Z}_i \rfloor, \tag{15}$$

where, Zi and \hat{Z}_i are the vectors of observed and forecasted values of the dependent variable at training stage, respectively;

- 2. Running test stage;
- 3. Combining errors of the training stage with predicted values of the test stage:

$$Z_p = \mathrm{K-NN}_{Z_i}(x_i) + \mathrm{K-NN}_E(x_i), \qquad (16)$$

where, K-NN_{Z_i}(x_i) is the predicted value of the dependent variable at the test stage, K-NN_{E_i}(x_i) is the error of the dependent variable at the training stage, and Z_P is the predicted value of the dependent variable at the test stage. The sizes of training and test datasets were considered 75% and 25%, respectively [14,26,27]; further, It has been tried to have both extreme and normal events in both training and test datasets to reflect the abilities of this proposed method, more realistically.

4. Case study

Zayandeh-rud River is the main water resource for terrestrial ecosystem, and agricultural and municipal consumptions of Esfahan City located in the centre of Iran; and Zayandeh-rud dam, with a volume of 1470 MCM, controls the streamflow of Zayandeh-rud River (Figure 1). Monthly data of inflow to Zayandehrud dam during a 30-year period from 1971 to 2001 is used at this study. Previous research in this area of study has identified that the accumulated 3-month streamflow of autumn and the average of Southern Oscillation climate Index (SOI) from summer to the end of autumn can be considered as the most appropriate

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Figure 1. The location of Zayandeh-rud dam basin.

predictor variables for forecasting the accumulated 9month inflow from winter to the end of the following summer [14,26].

Here, three goodness-of-fit criteria are employed in comparing the results. In the following equations, obs_i and for_i are the observed and forecasted values of the dependent variable, respectively, and n is the total number of samples (time spans):

1. Root of Mean Square Error (RMSE):

$$\text{RMSE} = \frac{\sqrt{\sum_{i=1}^{n} (obs_{i} - for_{i})^{2}}}{n}.$$
(17)

2. Volume Error (VE):

$$\% VE = \frac{\sum_{i}^{n} \left| \frac{obs_{i} - f \, or_{i}}{obs_{i}} \right|}{n}.$$
(18)

3. Correlation coefficient:

$$\operatorname{Corr}\% = \frac{Cov(obs, for)}{\sigma_{obs} \times \sigma_{for}},\tag{19}$$

where, Cov(obs, for) is the covariance between the observed and predicted values and σ_{obs} and σ_{for} are standard deviations of the observed and predicted values, respectively.

5. Results and discussion

In the current research, five data preprocessing functions, six distance functions, and three approaches (with 90 combinations) were applied for specifying the best number of neighbours and weights of predictors. Table 1 presents the best derived results amongst all the mentioned combinations with/without taking benefit from the proposed extrapolation method.

As for the Empirical method, due to the length of time series (30 time spans), the best number of neighbours was calculated 5 (k = 5). Further, considering the correlation between the predictors and dependent

Table 1. Final results of the best effective components of K-NN method for long-lead forecasting of inflow to Zayandeh-rud dam.

			Preprocessing functions	Distance functions	Weights of predictors		The best		Whole data		
		Methods			3-month streamflow of autumn	6-month SOI	no. of neighbours	Extrapolation method	CORR	% V	RMSE
st IS	reprocessing and distance functions	Empirical & trial-error processes	Max imum scaling	Euclidean	0.8	0.2	5	No	80	17	42
ioi ·								Yes	84	14	35
For the l combinat		Evolutionary optimization algorithm	Range scaling	Mahanalobis	0.63	0.37	6	No	92	10	34
	ч. ч.							103	50	0	20
orst ions ssing	of preprocessing o and distance functions	Empirical & trial-error processes	Profile	Cosine	0.8	0.2	5	No	65	31	54
For the w combinati of preproce		Evolutionary optimization algorithm	Profile	Lance-William	0.63	0.37	6	No	75	28	50

variable, weights of predictors were considered as 0.8 for accumulated autumn streamflow ($w_{\text{streamflow}} = 0.8$) and 0.2 for average of SOI from summer to the end of autumn ($w_{\text{SOI}} = 0.2$). In the trial-error method, weights were considered similar to those of the empirical method and then GCV was calculated for a range of k from 1 to 10.

According to Table 1, the best data preprocessing and distance functions for the empirical and trialerror processes were Maximum Scaling and Euclidean, respectively. RMSE, VE, and Corr for the abovementioned combination were derived 42, 17, and 80, respectively. With the same k and weights, the worst results of RMSE, VE, and Corr were evoked as 54, 31, and 65 for the combination of profile function as the data preprocessing function and cosine function as the distance function.

When evolutionary optimization algorithm of HBMO was used, the best effective component was presented as k = 6, $w_{\text{streamflow}} = 0.63$, $w_{\text{SOI}} = 0.37$, range scaling as the data preprocessing function, and

Mahanalobis as the distance function. RMSE, VE, and Corr for this combination were calculated 34, 10, and 92, respectively. With the same k and weights, the worst results had RMSE, VE, and Corr equal to 50, 28, and 75 for the combination of profile function as the data preprocessing function and Lance-William function as the distance function.

The positive influence of employing the proposed extrapolation method at K-NN is shown in Table 1. The results present the capability of this method to present more accurate forecasts, especially in case of the existing extreme events. The mentioned extrapolation method has improved the values of RMSE, VE, and CORR to 35, 14, and 84 for the Empirical and the Trial-Error process methods, as well as to 25, 8, and 96 for the HBMO method.

The results of goodness-of-fit criteria for the optimized K-NN in comparison with a regular K-NN presents an increase by 31% in CORR (from 65% to 96%), a decrease from 31% to 8% in VE, and finally a drop from 54% to 25% in RMSE. Figures 2 to 5



Figure 2. Final results based on the empirical and trial-error methods without applying the extrapolation method.



Figure 3. Final results based on the empirical and trial-error methods with applying the extrapolation method.



Figure 4. Final results based on HBMO method without applying the extrapolation method.



Figure 5. Final results based on HBMO method with applying the extrapolation method.

indicate the forecasts based on different approaches with/without considering the proposed extrapolation method. Final results present the increase in the accuracy of forecasts by using the proposed extrapolation method in comparison with common K-NN, especially for extreme events such as 1982, 1986-7, 1991, and 1997 to 2001. It is worth noting that even by using extrapolation method, the forecasts of maximum extreme events (e.g., 1992) are still underestimated, while the forecasts of minimum extreme events (e.g., 1997 to 2001) are overestimated, which shows the necessity of further research in this issue.

6. Summary, conclusion, and future research direction

This research aimed at showing the potentials, abilities, and disadvantages of K-NN method in long-lead streamflow forecasting of Zayandeh-rud River inflow to Zayandeh-rud storage reservoir from 1971 to 2001. A variety of combinations between preprocessing and distance functions along with different methods to estimate the best number of neighbours and weights of predictors at distance functions were considered to increase the accuracy of forecasts. Moreover, a proposed method was introduced and applied to decrease the errors of forecasts, especially for extreme events.

Overall, the results presented remarkable improvements: an increase by 31% in CORR (from 65% to 96%), a decrease from 31% to 8% in VE, and finally a drop from 54% to 25% in RMSE; however, it seems that the proposed extrapolation method has not been completely successful (underestimations of maximum extreme events and overestimations of minimum extreme events). However, finally, using more complicated methods such as HBMO in optimizing the best number of neighbours and weights of predictors at distance functions leads to growing the accuracy in terms of complexities and time consuming. It seems that Empirical methods can be considered as a serious competitive alternative. The latter point, besides introducing more effective extrapolation methods, is a topic which needs to be considered as a direction for future research.

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