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Application of GIS-based data driven random forest and maximum entropy models for groundwater potential mapping: A case study at Mehran Region, Iran

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ABSTRACT

Groundwater is considered as the most important natural resources in arid and semi-arid regions. In this study, the application of random forest (RF) and maximum entropy (ME) models for groundwater potential mapping is investigated at Mehran Region, Iran. Although the RF and ME models have been applied widely to environmental and ecological modeling, their applicability to other kinds of predictive modeling such as groundwater potential mapping has not yet been investigated. About 163 groundwater data with high potential yield values of ≥11 m^3/h were obtained from Iranian Department of Water Resources Management (IDWRM). Further, these selected wells were randomly divided into a dataset 70% (114 wells) for training and the remaining 30% (49 wells) was applied for validation purposes. In total, ten groundwater conditioning factors that affect the storage of groundwater occurrences (e.g. altitude, slope percent, slope aspect, plan curvature, drainage density, distance from rivers, topographic wetness index (TWI), landuse, lithology, and soil texture) were used as input to the models. Subsequently, the RF and ME models were applied to generate the groundwater potential maps (GPMs). Moreover, a sensitivity analysis was used to identify the impact of variable uncertainties on the produced GPMs. Finally, the results of the GPMs were quantitatively validated using observed groundwater dataset and the receiver operating characteristic (ROC) method. Area under ROC curve (AUC) was used to compare the performance of RF with ME. The uncertainty on the preparation of conditioning factors was taken in account to enhance the model. The validation results showed that the AUC for success rate of RF and ME models was 86.5 and 91%, respectively. In contrast, the AUC for prediction rate of RF and ME methods was obtained 83.1 and 87.7%, respectively. Therefore, RF and ME were found to be effective models for groundwater potential mapping.

1. Introduction

Groundwater is one of the most valuable natural resources serving as a major source of water to communities, agricultural and industrial purposes. Groundwater can be defined as water in saturated zone (Berhanu et al., 2014; Fitts, 2002) which fills the cracks in rock mass or pore spaces among mineral grains. Iran is considered an arid and semi-arid country which two-thirds of it landmass is classified as desert land. Therefore, groundwater is considered as the main source of the water supply for various uses in this country (Nosrati and Eeckhaut, 2012; Razandi et al., 2015). The agricultural sector in Iran is considered as one of the most important economic sectors of the country, and water crisis/scarcity is the most limiting factor for agricultural expansion and production (Zehtabian et al., 2010). Currently, groundwater and surface water resources supply about 65% and 35% of water consumed in Iran, respectively. The application of geographic information system (GIS)-based models for producing the groundwater potential map (GPM) and having knowledge on groundwater resources can be helpful, especially in data scarce areas (Adiat et al., 2012; Russo et al., 2015). From a groundwater potential productivity viewpoint, the 'groundwater potential' is defined as the possibility of groundwater occurrence in an area (Jha et al., 2010).

Generally, the occurrence and productivity of groundwater in a given aquifer is affected by several geo-environmental factors. These factors are topography, geological structure, fracture density, lithology, aperture and connectivity of fractures, secondary porosity, groundwater table distribution, slope degree, landform, drainage pattern, and land use (Mukherjee, 1996). The significant relationship

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of groundwater occurrence and conditioning factors has been indicated in Oh et al. (2011), Adiat et al. (2012), Lee et al. (2012b), and Pourtaghi and Pourghasemi (2014). The groundwater conditioning factors considered in this study are the altitude, slope percent, slope aspect, plan curvature, drainage density, distance from rivers, topographic wetness index (TWI), landuse, lithology, and soil texture.

The traditional approach of groundwater exploration using drilling, geophysical, geological, hydrogeological, and methods normally are costly, time consuming, and uneconomical (Israil et al., 2006; Jha et al., 2010; Todd and Mays, 1980). Recently, application of GIS and remote sensing (RS) techniques for groundwater potential mapping has become an effective procedure (Davoodi Moghaddam et al., 2015; Oh et al., 2011). GIS is a potentially effective tool to handle huge amount of spatial data and can be utilized in a number of fields such as water resources management and delineation of groundwater potential zones (Fashae et al., 2014; Rahmati et al., 2014, 2015). In recent years, different studies have been applied using GIS-based data driven models to produce the GPM (Dar et al., 2010; Madrucci et al., 2008; Prasad et al., 2008). In order to prepare the GPM, some studies have applied probabilistic models such as frequency ratio (FR) (Oh et al., 2011; Razandi et al., 2015), multi-criteria decision analysis (Chowdhury et al., 2009; Kaliraj et al., 2014; Pradhan, 2009; Rahmati et al., 2014) weights-of-evidence (WofE) (Corsini et al., 2009; Lee et al., 2012a; Ozdemir, 2011a; Pourtaghi and Pourghasemi, 2014), logistic regression (LR) (Ozdemir, 2011b; Pourtaghi and Pourghasemi, 2014), evidential belief function (EBF) (Mogaji et al., 2014; Nampak et al., 2014; Pourghasemi and Beheshtirad, 2014), certainty factor (CF) (Razandi et al., 2015), decision tree (DT) (Chenini and Mammou, 2010), artificial neural network model (ANN) (Lee et al., 2012b), and Shannon's entropy (Naghibi et al., 2014). Recently, Manap et al. (2014) applied FR model to map the groundwater potentiality in Kuala Langat, Malaysia. In the FR model, the study considered the relationship between groundwater occurrence and each conditioning factor separately, while not considering the relationships among all the conditioning factors themselves. Also, Adiat et al. (2012) used the analytic hierarchy process (AHP) for groundwater potentiality mapping in Kedah, Peninsula Malaysia. Machiwal et al. (2011) utilized the AHP method for spatial prediction of groundwater potentiality in Udaipur, India. Their results indicated that AHP requires questionnaires of comparison ratings to define the weights for the thematic layers in groundwater potentiality analysis. However, as stated in Matori (2012), this method requires expert knowledge and has many biases. The bivariate (e.g. FR, EBF, etc.) and multivariate (e.g. LR) statistical methods have some drawbacks for measuring the relationship between conditioning factors and groundwater occurrence, because of definition of statistical assumptions prior to the study (Tehrany et al., 2013; Umar et al., 2014). Furthermore, ANN and LR methods show a variety of problems such as the opacity of neural networks and their sensibility towards outlier values of logistic regression (Abrahart et al., 2008).

In contrast to the mentioned approaches, machine learning technique such as the random forest (RF) and maximum entropy (ME), which can handle data from various measurement scales and makes no statistical assumptions, was found useful for groundwater potential modeling. Major applications of the RF and ME models are found in environmental and ecological modeling (e.g. Ließ et al., 2012; Moreno et al., 2011; Oliveira et al., 2012; Oppel et al., 2011; Yost et al., 2008; Vincenzi et al., 2011), environmental sciences (Rodriguez-Galiano et al., 2014), eco-hydrological distribution modeling (e.g. Peters et al., 2007), landslide susceptibility mapping (Park, 2014; Youssef et al., 2015) and within the earth sciences in remote sensing (e.g. Gislason et al., 2006; Pal, 2005; Rodriguez-Galiano et al., 2012a, 2012b). However, no example of the use of the RF and ME models in groundwater potential modeling was found.

The RF and ME models offer new approaches to the groundwater potentiality mapping, as they are relatively robust to outliers and they can overcome the "black-box" limitations of ANNs, assessing the relative importance of the groundwater conditioning factor and being able to identify the most important factors and reducing dimensionality. Moreover, the parameterization of RF and ME models are very simple and they are computationally lighter than other machine learning techniques such as support vector machine (SVM) and ANNs (Rodriguez-Galiano and Chica-Olmo, 2012). At the other extreme, RF provides very good results compared to other machine learning techniques such as support vector machines (SVM) and ANN or to other decision tree algorithms (Breiman, 2001; Liaw and Wiener, 2002). Furthermore, Loosvelt et al. (2012) demonstrated that uncertainty estimates can be easily assessed when RF is applied in the modeling. Kuhnert et al. (2010) stated that RF presents a very hopeful model for a wide range of environmental issues due to their adaptability, flexibility, relatively simple interpretability and performance. Although RF and ME models are being currently applied as remote sensing data classifier and ecological model, respectively, their potential as a spatial modeling tool for producing the GPM are still underexplored due to their novelty.

The main aim of current study is to apply RF and ME models for groundwater potential assessment, and for this purpose, Mehran Region in western Iran was selected. As stated, RF and ME models don't define strict assumptions prior to study which is considered as a strong advantage of such approaches and can also handle data from various measurement scales. The main difference between this study and the approaches described in the aforementioned publications is that the RF model is applied and the result is compared with ME model in the study area. The RF and ME models are new in the area of groundwater potential mapping compared to other methods. Because no such studies have been published so far in the study area, therefore, the current research is the pioneer work in this subject which is crucial for rapid generation of GPM. Hence, the result of GPM can be useful for planners in the natural resource management and comprehensive evaluation of groundwater potential for future planning. The specific objectives of this study are to (1) explore the capability of RF and ME models for groundwater potential mapping, (2) analyze the importance of groundwater conditioning factors, and (3) compare the performance of RF and ME models for accurate groundwater potential mapping.

2. Material and methods

Fig. 1 depicts the methods and the flow chart used in this study.

2.1. Study area description

The Mehran Region is situated in the northern part of Iran, between 33° 2′ to 33° 8′ N latitudes, and 46° 03′ to 46° 23′ E longitudes (Fig. 2). It covers an area of approximately 226km^2.The land surface elevation in the study area varies from 91 to 271 m above sea level, with a mean elevation of 105 m. The terms of "aridity" and "semi-aridity" are relative and range of these terms should be defined for any area. According to the climatic classification in Iran, arid and semi-arid are regions receive annual precipitation of less than 100 mm, and 100–400 mm, respectively. Thus, the study area is considered to have a semi-arid climate with an average annual rainfall of 320 mm (IDWRM, 2013). The study area receives about 85% of its annual rainfall from December to April. In winter, temperature ranges from −8 to 10.5 °C while in summer; it varies from 25 to 39 °C.

Geologically, the study area is located in Zagros structural zone of Iran. The Zagros is considered as a region of poly-phase deformation, fracture systems, and the latest reflecting the collision of Eurasia and Arabia (Alavi, 1994). The aquifer of Mehran Region is reported as an unconfined in nature and is recharged across its entire surface by infiltrating rainfall and streams leaking into the subterranean system. Exploitation of groundwater resources in this area includes deep and semi-deep wells, and springs. It is evident that the general groundwater

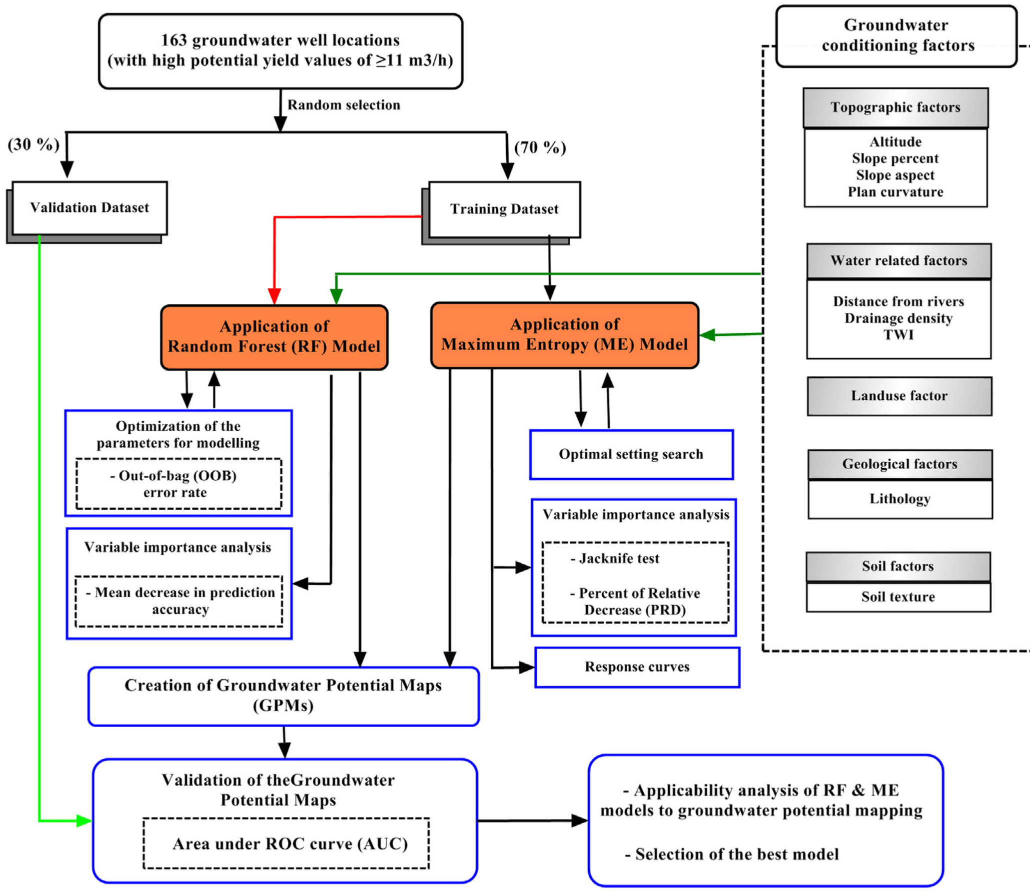

Fig. 1. Methodology flowchart used in this study.

flow direction is from the eastern region of the aquifer to the western regions of the aquifer, and the general topographic gradient of the plain is east to west. The groundwater assessment is very important within this region, since groundwater supplies irrigation and drinking water requirements. Also, the people living in this region depend on dry farming and irrigated agriculture.

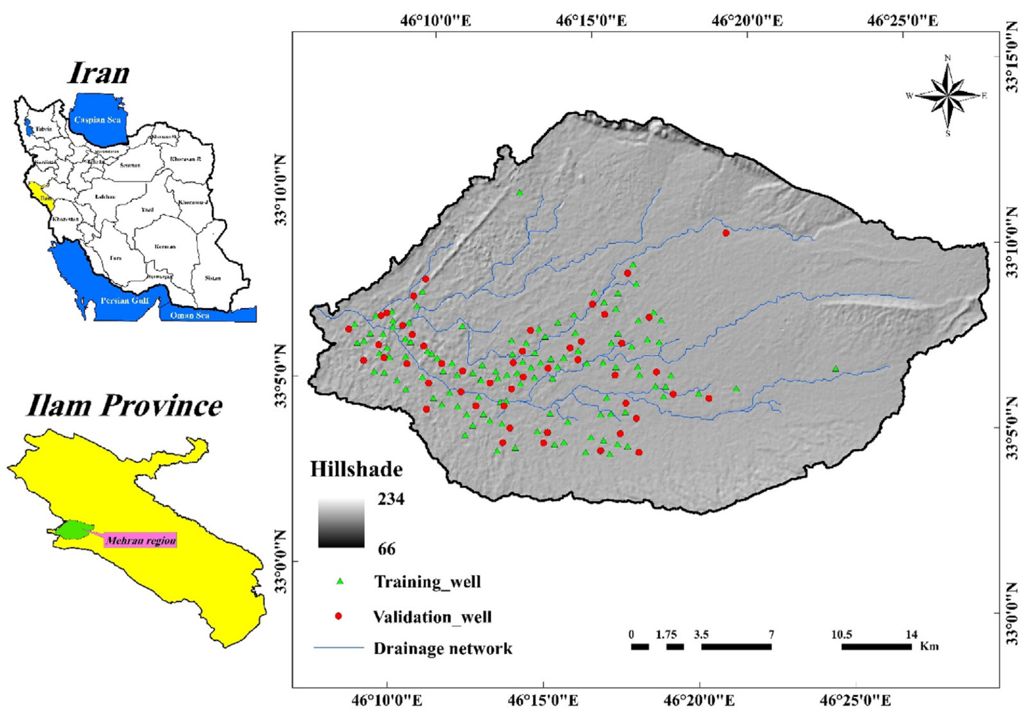

Fig. 2. Groundwater well locations map with the hill-shaded map of Mehran Region, Iran.

2.2. Dataset used

2.2.1. Groundwater well inventory map

The groundwater information (i.e. number of wells, yield, depth, etc.) was compiled from the Iranian Department of Water Resources Management (IDWRM). Groundwater yield is based on actual pumping test analysis of groundwater in the study area, and also, the groundwater potential is based on prediction of the best potential for groundwater extraction.

According to previous studies and groundwater productivity reports of IDWRM, only groundwater data with high potential yield of ≥ 11 m^3/h were selected. This groundwater wells data (163 groundwater well locations) were divided using a random partition algorithm for a training (70% of the dataset, 114 wells) and validation (30% of the dataset, 49 wells). Fig. 2 illustrated both the training dataset and validation dataset locations in the study area.

2.2.2. Geo-environmental factors influence on groundwater occurrences

The main geo-environmental factors considered in the present study, which are influential to the groundwater occurrence, are described in Table 1.

2.2.2.1. Topographic factors. The digital elevation model (DEM) was created by digitizing contour lines (20 m interval) and surveying of base points. We used the ArcGIS TIN (Triangular Irregular network) module, and then converted the TIN to Raster (pixel size 20 m). The contour lines and points were prepared by Iran's National Cartographic Center (NCC), and this study only created the DEM from these layers. The DEM was applied to derive different topographic factors such as altitude (Fig. 3a), slope percent (Fig. 3b), slope aspect (Fig. 3c) and plan curvature (Fig. 3d) using ArcGIS10.2 software.

2.2.2.2. Water related factors. Various factors such as drainage density, distance from rivers, and topographic wetness index (TWI) play significant roles in groundwater movement, recharge and hydrogeological systems. Using the DEM, the distance from rivers (Fig. 3e) and drainage density (Fig. 3f) were produced in a GIS environment. The TWI as a secondary topographic index has been widely used to illustrate the impact of topography/morphology conditions on the location and size of saturated source zones of surface runoff generation. Recently, TWI has been applied for groundwater potential mapping (Pourtaghi and Pourghasemi, 2014; Razandi et al., 2015) describing spatial wetness patterns. It can be calculated as follows (Moore et al., 1991):

$$TWI = \ln\left(\frac{\alpha}{\tan\beta}\right) \tag{1}$$

where α is the cumulative upslope area draining through a point (per unit contour length) and tanβ is the slope angle at the point. In this study, TWI map was prepared in SAGA-GIS (System for Automated Geoscientific Analyses) (Fig. 3g).

2.2.2.3. Landuse. The landuse map of the study area was prepared from Landsat Enhanced Thematic Mapper plus (ETM^+) image (May 27, 2013) through supervised classification using maximum likelihood algorithm, and false color composite (FCC) techniques in ENVI 4.2 software. The accuracy of landuse map was assessed using a set of 350 sampled field points. Ground-truthing was employed to produce a confusion matrix and to calculate overall accuracy. Land cover classification accuracy assessment procedure is explained in detail in several publications (e.g. Congalton, 1991; Lillesand and Kiefer, 2000; Foody, 2002). The produced landuse map indicates overall accuracy of 85.3%. The landuse map of the study area is illustrated in Fig. 3h. Four landuse classes were generated from the classification: agriculture, urban, range, and forest areas.

Table 1
The spatial database construction.

Classification	Sub-classification	Data type	Scale
Groundwater base map	Tube well	Point	1:25,000
	Topographic map	Point, line, and polygon	1:50,000
	Land use map	Grid	20 × 20
	Geological map	Polygon	1:100,000
	Soil texture map	Grid	20 × 20

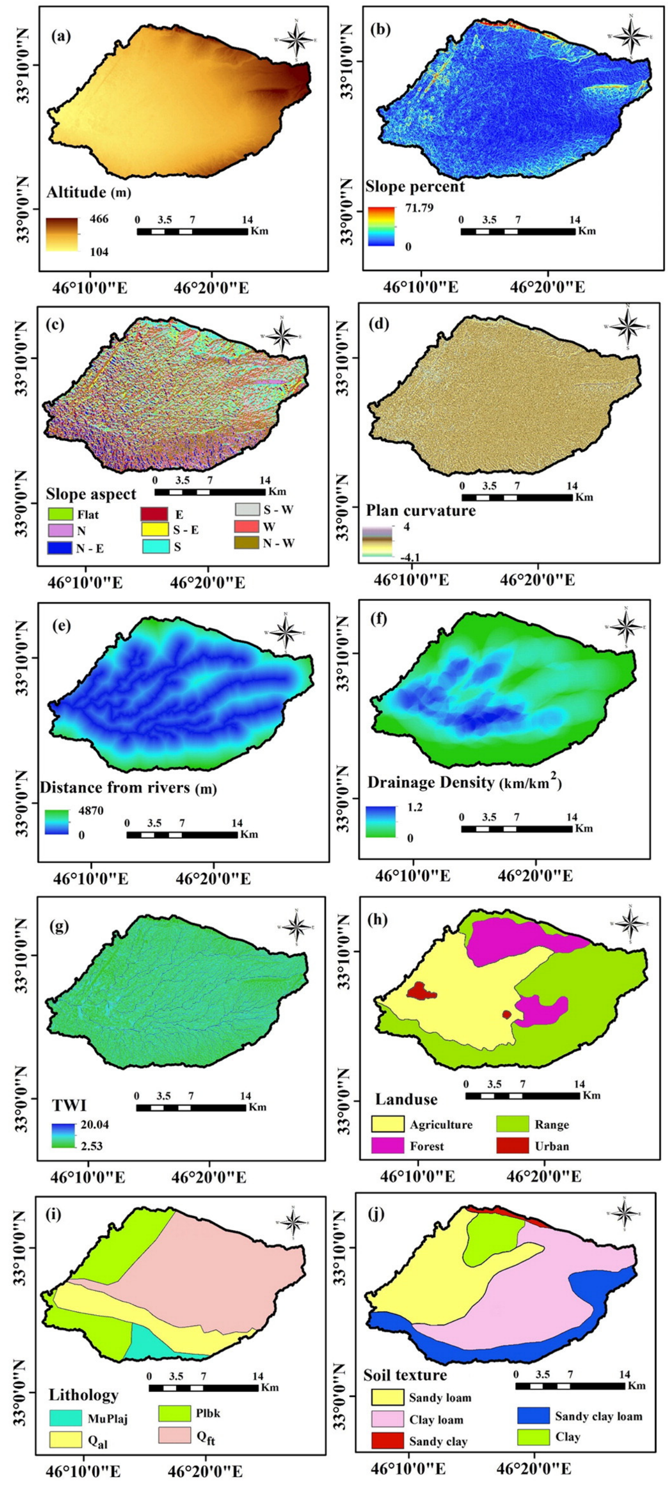

Fig. 3. Groundwater conditioning factors: (a) altitude, (b) slope percent, (c) slope aspect, (d) plan curvature, (e) drainage density, (f) distance from rivers, (g) TWI, (h) landuse, (i) lithology, and (j) soil texture.

2.2.2.4. Geological factors. The lithology is considered as one of the most important indicators of hydrogeological features which play a fundamental role in both the porosity and permeability of aquifer materials (Ayazi et al., 2010; Charon, 1974). The analog lithology map (1:100,000) was obtained from the Geological Survey of Iran (GSI) and the digital lithology map was generated using ArcGIS 10.2 (Fig. 3i). According to Geological Survey of Iran (GSI, 1997), the lithology of the study area is varied (Table 2), and covered by red marl and sandstone (MuPlaj), conglomerate locally with sandstone (Plbk), conglomerate marly and sandy conglomerate with calcareous and clay matrix (Bk), stream channel and flood plain deposits (Q_{al}), and high level pediment fan and valley terrace deposits (Q_{ft}).

2.2.2.5. Soil texture. Soil texture is one of the most important factors in the surface and subsurface runoff generation and infiltration process (Mogaji et al., 2014). The soil texture map was obtained from the Iranian Department of Water Resources Management (IDWRM). There are four classes of soil texture in the study area: sandy loam, clay loam, sandy clay, sandy clay loam, and clay (Fig. 3j).

2.3. Description of the models

2.3.1. Random forest model

2.3.1.1. Basic principle of Random Forest algorithm. Random forest (RF) is a nonparametric technique (Breiman, 2001) that was developed as an extension of classification and regression trees (CART) and generates many classification trees (Breiman et al., 1984) to improve the prediction performance of the model. During the RF modeling, each split of the tree is determined using a randomized subset of the variables/factors at each node. The final outcome of model building process is the average of the results of all the trees (Cutler et al., 2007). To run the RF model, it was necessary to define a priori two parameters: the number of variables/factors to be used in each tree-building process (m_{try}) and the number of trees to be built in the forest to run (n_{tree}). In order to minimize the generalization error, the mentioned parameters should be optimized. Breiman (2001) and Liaw and Wiener (2002) stated that even a variable/factor ($m_{try} = 1$) can generate good accuracy, while Gromping (2009) proves the need to include at least two variables/factors (i.e. $m_{try} = 2, 3, 4,\ldots, m$) in order to avoid using the weaker regressors as splitters.

The RF model consists of a combination of numerous trees, where each tree is generated by bootstrap samples, leaving about one-third of the overall sample for validation, using the out-of-bag (OOB) error. As discussed in Breiman (2001), the OOB error is an unbiased estimate of the generalization error. The main advantages that arise from this method are: (a) no overfitting, (b) low bias and low variance due to averaging over a large number of trees, (c) low correlation of individual trees since the diversity of the forest is increased through the usage of a limited number of variables/factors, (d) robust error estimates using the OOB data, and consequently, and (e) higher prediction performance (Prasad et al., 2006; Wiesmeier et al., 2011).

The variance and covariance between grid cells can be computed using OOB error data (Kuhnert et al., 2010; McKay and Harris, 2015). These components denote a measure of the uncertainty around the estimate of groundwater potentiality at a grid cell.

Table 2
Lithology of the Mehran Plain, Iran.

Code	Lithology	Formation	Geological age
MuPlaj	Red marl and sandstone	Aghajari	Miocene
Plbk	Conglomerate locally with sandstone	Bakhtyari	Pliocene
Q_{al}	Stream channel and flood plain deposits	–	Quaternary
Q_{ft}	High level pediment fan and valley terrace deposits	–	Quaternary

A detailed description of the mathematical formulation of RF model is found in Breiman (2001); Liaw and Wiener (2002). The aim of RF is to identify the suitable model to analyze the relationship between independent variables and a dependent variable in the calibration phase (i.e. model building) to determine the weight value for each factor. In this study, groundwater wells of training dataset (i.e. 114 groundwater wells), and 10 groundwater conditioning factors (i.e. altitude, slope percent, slope aspect, plan curvature, drainage density, distance from rivers, topographic wetness index (TWI), landuse, lithology, and soil texture) were used as dependent variable and independent variables, respectively.

2.3.1.2. Variable importance analysis and generation of groundwater potential map. In this study, the RF model was used to examine relationship between groundwater conditioning factors and groundwater occurrence, and to predict the groundwater potentiality. The parameter *mtry* was determined via the internal RF function TuneRF that recognizes the optimal number of factors. Another advantage of the RF model is that it allows investigation of the variable importance (contribution of each variable) measured by the mean decrease in prediction accuracy (%IncMSE). Therefore, mean decrease in prediction accuracy and cross-validation were used to evaluate random forests and to examine them on the propagation of uncertainty due to uncertain groundwater conditioning factors (Peters et al., 2007, 2009; Naghibi and Pourghasemi, 2015).

In this study, the “randomForest” package of R open source software (R Development Core Team, 2015) was used for all RF modeling, then the final produced map was brought into ArcGIS to produce the groundwater potential map (GPM).

2.3.2. Maximum entropy model

2.3.2.1. Basic principle of maximum entropy modeling. Phillips et al. (2006) proposed the maximum entropy (ME) model specifically designed for ecological modeling and species distribution assessment, when only presence data are available for modeling. Graham et al. (2008) stated that the ME model is more robust to spatial errors in occurrence data and applies the presence only datasets to predict the suitability of habitat or the potentiality of phenomena. The ME model is based on a machine-learning response that makes spatial predictions from incomplete data (Medley, 2010; Moreno et al., 2011). The ME model is also deterministic and converges to probability distribution of the maximum entropy (Baldwin, 2009; Berger et al., 1996). For groundwater potential mapping, the model starts with a uniform distribution, and performs a number of iterations based on the most significant geo-environmental factors until no further improvements in the spatial prediction are made (Phillips et al., 2004, 2006). The goal of ME model is to identify the probability distribution (Φ) of target occurrences over the set locations X within the study area. Conditioning factors are used to define the moment constraints on the probability distribution (Φ). The moment, such as the mean, is obtained from the values of the conditioning factors at all groundwater well locations (with high productivity). By applying the ME algorithm, the most uniform distribution is recognized and selected from among many possible distributions (Phillips and Dudík, 2008).

In the current study, only the salient aspects of the ME model for modeling are given, synthesized from Phillips et al. (2006), and Elith et al. (2011). Let $\mathbf{x}$ denotes a random site/pixel over the study area and $\Phi(\mathbf{x})$ (non-negative and sums to one) be value of the target probability distribution at location $\mathbf{x}$. By applying Bayes' rule, the probability that the target is present at location $\mathbf{x}$, denoted as $P(y = 1|\mathbf{x})$ is expressed as shown (Park, 2014; Phillips et al., 2006):

$$P(y = 1|\mathbf{x}) = \frac{P(y = 1)P(\mathbf{x}|y = 1)}{P(\mathbf{x})} = \frac{P(y = 1)\ \Phi(\mathbf{x})}{1/_{|\mathbf{X}|}} \tag{2}$$

where $P(y = 1)$ and $|X|$ are the prevalence of target occurrences, and the number pixels or locations over the study area, respectively. $\Phi(\mathbf{x})$ estimated by the ME algorithm is equal to a Gibbs probability distribution (Phillips and Dudík, 2008; Phillips et al., 2006). As discussed in Phillips et al. (2006), the Gibbs probability distribution is indicated as (Eq. (3)):

$$q_\lambda(\mathbf{x}) = \frac{1}{Z_\lambda(x)} \exp\left(\sum_{i=1}^{n} \lambda_i f_i(\mathbf{x})\right), \tag{3}$$

Where.

$$Z_\lambda(x) = \sum_y exp\left(\sum_i \lambda_i f_i(x, y)\right), \tag{4}$$

where $Z_\lambda(x)$ and λ_i are a normalization constant (to make sure $q_\lambda(\mathbf{x})$ sums to one across the study area), and the vector of weights assigned to the features, respectively.

In the estimation phase of $q_\lambda(\mathbf{x})$, ME modeling tries to identify the distribution closest to the constraints using l_1 regularization to avoid over-fitting. Therefore, ME model aims to find the Gibbs probability distribution that maximizes the penalized log likelihood values (Park, 2014; Yost et al., 2008). Also, if there are m occurrences in the study area, the difference between regularization and log likelihood, which should be maximized, is denoted as $\Psi(\lambda)$ and expressed as (Phillips and Dudík, 2008):

$$\Psi(\lambda) = \frac{1}{m}\sum_{i=1}^{m} \ln(q_\lambda(\mathbf{x}_i)) - \sum_{j=1}^{n} \beta_j |\lambda_j| \tag{5}$$

where β_j is the regularization parameter for the j_{th} feature (f_j).

All input conditioning factors are introduced as random variables of the model according to the ME algorithm described by Convertino et al. (2014) that represent their uncertainty. Further, the variance of the estimation error characterizes the uncertainty associated with the estimated values, which is provided by ME model based on the upper and lower limits of the interval data, Bayes' rule, and Gibbs probability distribution (Douaik et al., 2005). The detailed explanation of mathematical formulation of this model is shown in Phillips et al. (2006) and Phillips and Dudík (2008).

2.3.2.2. Spatial sensitivity analysis and generation of groundwater potential map. Implementation of ME model to groundwater potential modeling, and the construction of prediction rate were done using the Maxent software (version 3.3.3 k). The prediction accuracy model can be examined using the receiver operating characteristic (ROC) curve. In this method, the area under the ROC curves (AUC) can measure the prediction accuracy qualitatively (Maier and Dandy, 2000; Tien Bui et al., 2012). Here, the groundwater well samples (training and validation datasets) were prepared in Excel format, and the conditioning factors were converted from raster to ASCII format, which is required in Maxent software. During the ME model run, 114 (70%) of the groundwater wells are randomly chosen using random selection algorithm for model training in the calibration phase. ME model is a popular machine learning technique that allows for examination of the relationship between a dependent variable and several independent variables that in our work are groundwater occurrence (114 groundwater wells) and 10 groundwater conditioning factors, respectively. The main output of the ME model is a groundwater potential map (GPM), where each pixel is assigned a presence probability value. Overall, before the generation of the GPM, optimal settings are first searched by predictive performance measures that affect the predictive performance and processing time significantly. These optimal settings are: the number of background samples and the best feature selection for continuous data representation (Phillips and Dudík, 2008). In this study, the optimal settings have been determined, the GPM is produced and interpretation of the results is down.

Uncertainty in the preparation of input layers is unavoidable (Janssen et al., 1994; Saltelli et al., 2000), and analyzing the variability of model output due to incomplete knowledge of real world situations simulated in models is important. Knowledge on the uncertainty of input data allows for a better interpretation of the model predictions (Helton and Davis, 2002; Loosvelt et al., 2012). A thorough review of 14 methods commonly used in uncertainty assessment such as data uncertainty engine, error propagation equations, inverse modeling (parameter estimation), inverse modeling (predictive uncertainty), expert elicitation, extended peer review, Monte Carlo analysis, NUSAP, multiple model simulation, quality assurance, stakeholder involvement, sensitivity analysis (SA), scenario analysis, and uncertainty matrix can be found in Refsgaard et al. (2007). Further, previous studies (Hamby, 1994; Archer et al., 1997; Crosetto and Tarantola, 2001; Chen et al., 2010) have been used SA as exploratory technique to describe the effect of variable variations on model outputs, allowing then a quantitative assessment of the relative importance of uncertainty sources (Ravalico et al., 2010). Saltelli et al. (2008) defined SA in terms of the study of how uncertainty in the model output can be apportioned to different sources of uncertainty in the input factors. In other words, SA investigates the contribution of each input factor to the uncertainty of the model outputs (Crosetto et al., 2000; Convertino et al., 2014). In our study, to assess the uncertainty of groundwater potentiality prediction using the SA, a Jackknife test was conducted for examining the effects of removing any of the conditioning factors on the potentiality map (Yost et al., 2008). At the other extreme, the Jackknife test can be considered to access the factors contribution (i.e. relatively importance) to the modeling (Park, 2014; Phillips et al., 2006). The percent of relative decrease (PRD) of AUC values as a percentage was also calculated to investigate the dependency of model output on the influence of conditioning factors using the following equation (Eq. 6) (Park, 2014):

$$PRD = \frac{(AUC_{all} - AUC_i)}{AUC_i} \times 100 \tag{6}$$

where AUC_{all} and AUC_i indicate the AUC values obtained from the groundwater potential prediction using all conditioning factors and the prediction when the ith conditioning factor has been excluded, respectively.

The PRD provides a complete characterization of the factor contribution and sensitivity analysis of the ME model that influences on the prediction accuracy and uncertainty level. Moreover, a response curve is also used to quantify the behavior of variables and to recognize relationships between each conditioning factor and the groundwater potential modeling.

Even if we demonstrate that machine learning methods such as ME model generate more accurate prediction, it is still important to identify the main sources of variation and factor contribution analysis that affect the uncertainties. Uncertainty in GPM predictions has two main different sources: (i) deficiencies of data quality (e.g. small sample sizes, missing covariates, biased and absent data), and; (ii) errors in the structural nature and specifications of the model. Thus, a more detailed assessment of the sources of uncertainties is important to improve the performance of groundwater potential modeling. The use of ME model can be important because it allows mapping the variance components and to evaluate the uncertainties (Diniz-Filho et al., 2009; Convertino et al., 2014), giving more information on where more research is needed to minimize variance.

The GPM for each model was classified according to four classification techniques in GIS environment, namely Natural Breaks, Quintile, Equal Interval, and Geometrical Interval, into four different groundwater potentiality zones, including low, medium, high, and very high. By comparing the results of each classification technique and the distribution of training and validation groundwater wells on the high and very high groundwater potentiality zones, it was found that the Quantile classification technique gave the most accurate distribution (Fig. 4). This agrees with Nampak et al. (2014), Naghibi and Pourghasemi (2015), and Razandi et al. (2015) in that Quantile classification technique is a good classifier in groundwater potentiality mapping.

2.3.3. Validation of groundwater potential maps

Validation step is the most important process of modeling and without it; the groundwater potential models will have no scientific significance (Chang-Jo and Fabbri, 2003). In groundwater potentiality assessment, the prediction accuracy of the applied models should be assessed by comparing the acquired GPM with existing groundwater yield data (validation dataset). The receiver operating characteristic (ROC) curve has been broadly applied in several researches to quantitatively evaluate the efficiency of potentiality mapping (Althuwaynee et al., 2014; Nampak et al., 2014; Park et al., 2014; Umar et al., 2014). The ROC curve is a scientific technique of describing the efficiency of probabilistic and deterministic detection and forecast systems (Swets, 1988).

Multiple hydrological and hydrogeological processes, operating at different temporal and spatial scales, are expected to influence the groundwater potentiality, and some of these processes are poorly recognized in the machine learning models. Consequently, there are several sources of uncertainty in the GIS-based data driven models that have been assessed in previous studies. In addition, some of the methodological uncertainties may arise because of statistical methods and differences in data sources used for potentiality modeling (Heikkinen et al., 2006). Zipkin et al. (2012) demonstrated that area under the ROC curve (AUC) is helpful in quantifying the uncertainty in model predictions while can account for detection biases associated with estimation. Here, the ability and uncertainty of RF and ME models in groundwater potential mapping have been investigated through the use of the AUC (Lin et al., 2015). To examine the efficiency and reliability of the GPM, both the success-rate and prediction-rate curves were calculated. As discussed in Yesilnacar (2005), the quantitative–qualitative relationship between the AUC and prediction accuracy can be classified as follows: 50–60% (poor), 60–70% (average), 70–80% (good), 80–90% (very good), and 90–100% (excellent).

3. Results and discussion

3.1. Application of random forest model

3.1.1. Selection of optimal parameters for random forest model calibration

As demonstrated in the study carried out by Breiman (2001), the out-of-bag (OOB) error rate is a helpful estimator of the generalization error depending on the number of trees. Therefore, the OOB as an unbiased procedure were used to select the optimum parameters of random forest algorithm (Goetz et al., 2015; Trigila et al., 2015) (Fig. 5). As seen in Fig. 5, the OOB error is a function of the number of trees, hence, reduced when more trees are added to the random forest algorithm. Based on this analysis, with the OOB equal to 0.215, *mtry* and *ntree* were obtained 3 and 1000, respectively.

3.1.2. Estimating independent variables importance

To assess the uncertainty of the GPM result as well as factors importance, we applied RF model described previously (Goetz et al., 2015). Fig. 6 shows the ranking of conditioning factors by their importance. As depicted in Fig. 6, the most influencing conditioning factors on groundwater occurrence were altitude, drainage density, lithology, and landuse. For other semi-arid regions in the worldwide, Rahmati et al. (2014); Nampak et al. (2014), and Razandi et al. (2015) also highlighted the importance of mentioned factors in producing the groundwater potential map (GPM). In decreasing order of importance, the other factors included in the RF model were: distance from rivers,

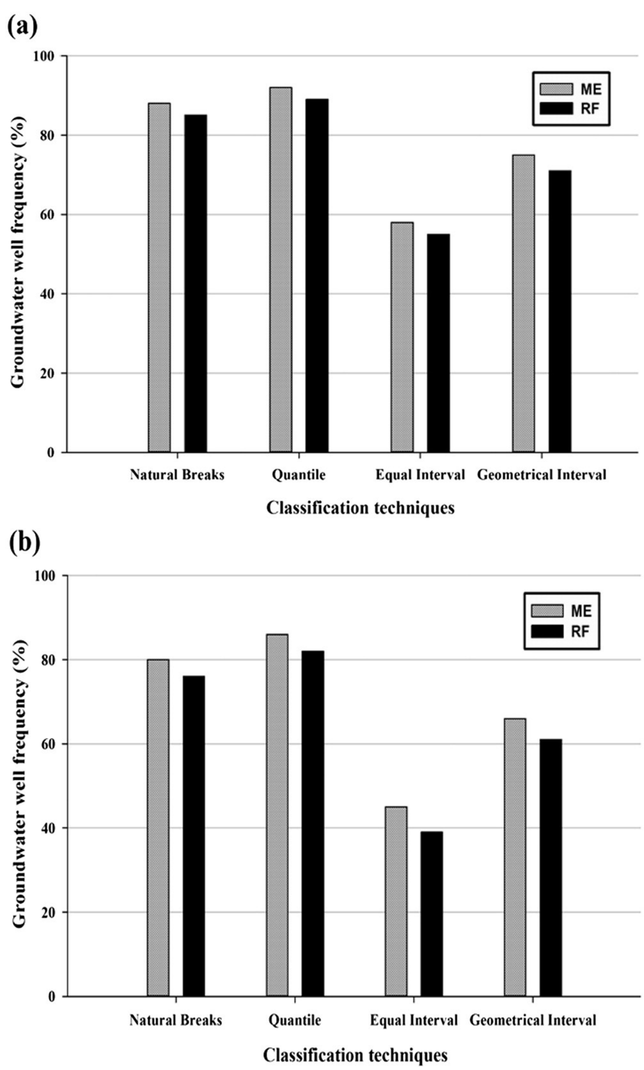

Fig. 4. The relationship between potentiality classes (High + Very high) and the percent frequency of groundwater wells (**a**) training and (**b**) validating groundwater well numbers of different classification techniques for RF and ME models.

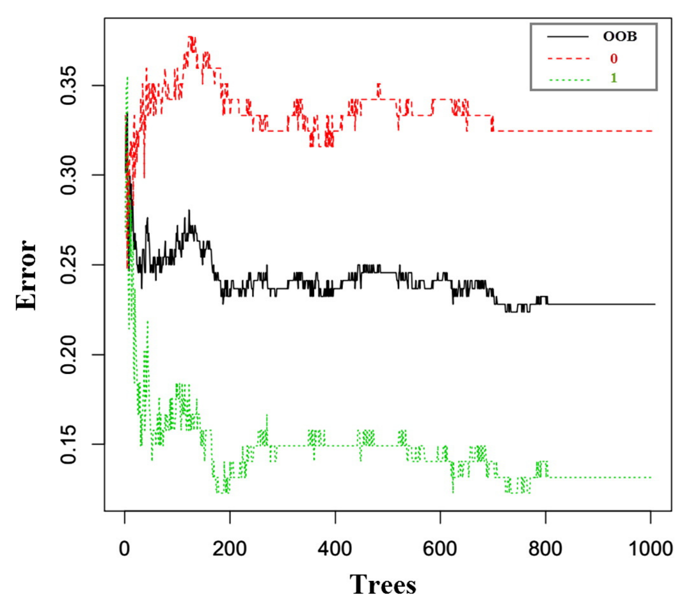

Fig. 5. Optimization number of trees based on OOB estimates of the error rate in RF model.

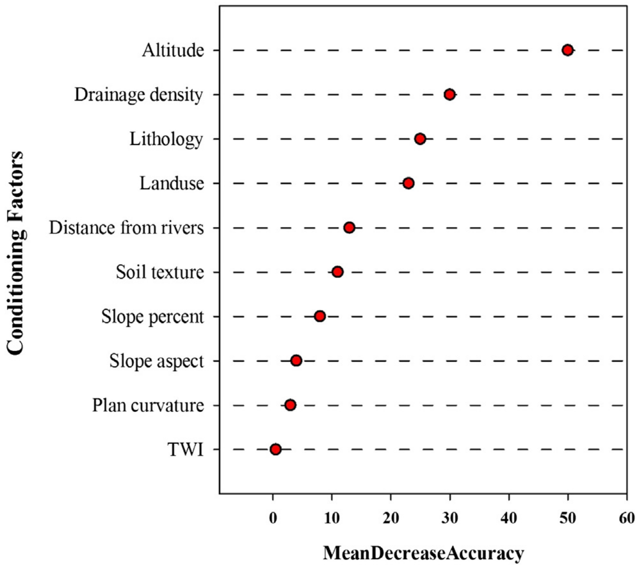

Fig. 6. Variables importance derived from RF model.

soil texture, slope percent, slope aspect, plan curvature and TWI. Therefore, slope aspect, plan curvature, and TWI factors are relatively weak predictors in comparison with other conditioning factors.

3.1.3. Groundwater potential mapping by RF model

As explained in RF methodology section, the GPM of Mehran Region, Iran was produced using RF model. Groundwater potential map derived from RF model is shown in Fig. 7. Visually, highest groundwater potentiality of Mehran Region is located on the center and western parts of the study area.

3.2. Application of maximum entropy model

3.2.1. Analyzing the response curves

Fig. 8 illustrates the response curves for ten groundwater conditioning factors used for groundwater potential assessment. The relationships between topographic factors and groundwater occurrence are as follows. In the altitude and slope percent maps, most groundwater occurred in the range of altitude between 100 and 150 m, and slope percent between 0 and 5, in which most plain areas are located. So, with increasing altitude and slope percent, the groundwater potentiality values decreased drastically. Therefore, areas close to low altitude and slope percent with large potentiality values could be separated from other locations, and the greatest contribution to spatial prediction could be obtained. In the response curve of drainage density, most groundwater occurred in the range of drainage density between 0.8 and 1 km/km^2. However, groundwater potentiality decreased in the areas with very high drainage density (i.e. increase the runoff transport capacity of drainage network). With regard to the distance from rivers, most groundwater occurred very close to rivers owing to an increase in the degree of groundwater recharge. The main aquifer recharge sources are precipitation and rivers.

Overall, the contributions of continuous data (except TWI factor) were strong, but some of the categorical layers including slope aspect, and plan curvature were relatively very weak. The lithology was the most influential factor among the five categorical data sets and the next dominant factors were landuse and soil texture. The lithology layer includes four classes and therefore, some lithological unites (e.g. Q_{al}, Q_{ft} and Plbk) with high potentiality could be separated from other lithological classes. In the case of the landuse type, agriculture and urban areas exhibited relatively higher potentiality values. It can be interpreted that irrigation water in addition infiltrates back to the groundwater system. In the soil texture map, most groundwater wells (with high yield productivity) observed in the sandy loam, and clay loam areas generally exhibited relatively higher potentiality values.

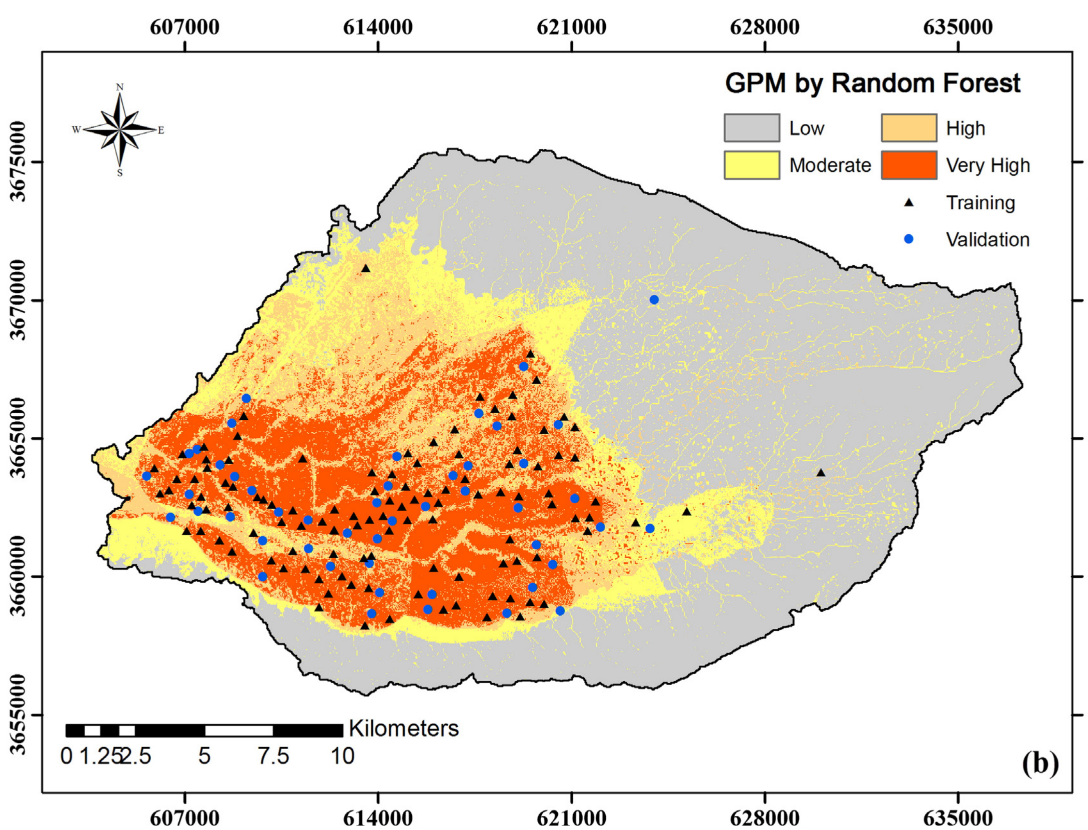

Fig. 7. Groundwater potential map produced by RF model.

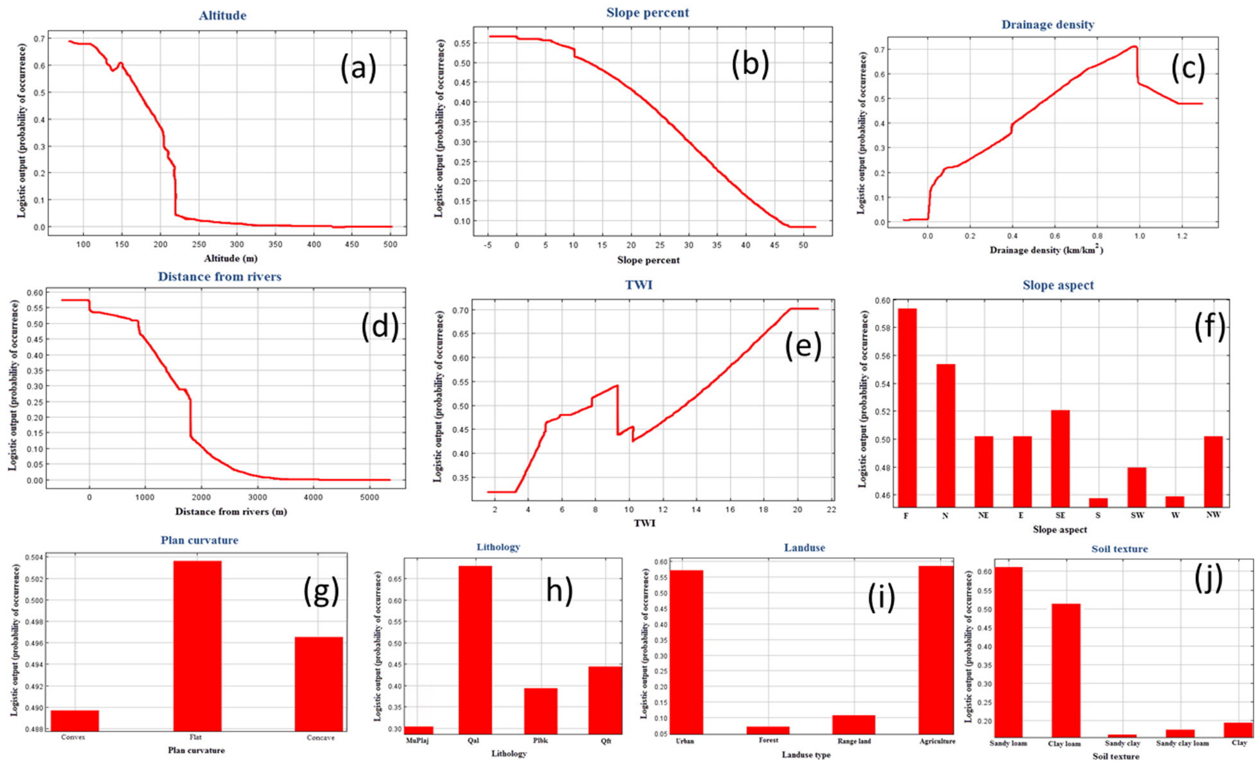

Fig. 8. Response curves for each conditioning factor.

Consequently, a relatively higher contribution for groundwater potential prediction was obtained among the five categorical data sets. However, these lesser contributions of some categorical layers did not mean that the categorical data layers were useless for groundwater potential mapping. As discussed in Park (2014), all these categorical layers did affect the final prediction result when simultaneously considered with continuous data sets.

3.2.2. Sensitivity analysis

Model input layers sets inevitably contain some uncertainties. To investigate the conditioning factor with the strongest effect on the result of groundwater potential prediction and to assess these uncertainties, a sensitivity analysis (Moreno et al., 2011; Park, 2014) was implemented. The test results in Table 3 are summarized as percent of relative decrease (PRD) of AUC value (i.e., loss of performance). The conditioning factors that most decreased the gain when these were omitted were the altitude (PRD = about 11), lithology (PRD = 6.46), drainage density (PRD = 5.89), landuse (PRD = 5.32), distance from rivers (PRD = 3.04), and soil texture (PRD = 2.47) which therefore appeared to have the most information that were not present in the other factors. Conversely, a few of the factors contributed weakly to the spatial prediction of groundwater potential, namely slope percent (PRD = 0.76), slope aspect (PRD = 0.76), plan curvature (PRD = 0.19), and TWI (PRD = 0.07) (Table 3). These results implied that the GPM is highly sensitive to altitude, lithology, drainage density, landuse, distance from rivers, and soil texture; however, it is less sensitive to slope percent, slope aspect, plan curvature, and TWI. Therefore, as stated by Convertino et al. (2014), SA allows managers and modelers to identify the conditioning factors (i.e. input variables) that reduce the variance of the model output to the most, which is considerably important in understanding the model structure.

Table 3
The Jackknife test results of variables when each factor is excluded in ME model.

Excluded factor	Decrease of AUC	Percent of relative decrease (PRD) of AUC
Altitude	9.67	11.02
Lithology	5.67	6.46
Drainage density	5.17	5.89
Landuse	4.67	5.32
Distance from rivers	2.67	3.04
Soil texture	2.17	2.47
Slope percent	0.67	0.76
Slope aspect	0.67	0.76
Plan curvature	0.17	0.19
TWI	0.07	0.07

3.2.3. Groundwater potential mapping by ME model

The groundwater potential map (GPM) in the study area was produced using both continuous and categorical data sets with 10,000 background samples. Finally, the GPM generated by the ME model and reclassified into four zones, namely, 'low', 'moderate', 'high', and 'very high' groundwater potentiality is shown in Fig. 9. In the GPM, the highly potential areas are found in the western and central parts of the study area, where the landuse and lithology types are agriculture and Q_{al} and Q_{ft} classes, respectively. Overall, the gently sloping areas which are also located in Q_{al} and Q_{ft} lithological classes, and near rivers showed high groundwater potentiality. On the other hand, the steeply sloping areas consisting of MuPlaj (i.e. Red marl and sandstone), and Plbk (i.e. conglomerate locally with sandstone) classes showed the lowest potentiality values.

3.3. Model performance and comparison between RF and ME models

Figs. 10a and 11a show the success-rate curve of RF and ME models that AUC were 86.5% and 91% of success accuracy, respectively. Since the success-rate curve used the training dataset that have already been used during the RF modeling, thus the success-rate curve is not a suitable technique for examination of the prediction capability of the model (Pradhan, 2013). However, this curve may help to illustrate how well the resulting GPM has classified the areas of existing wells. On the

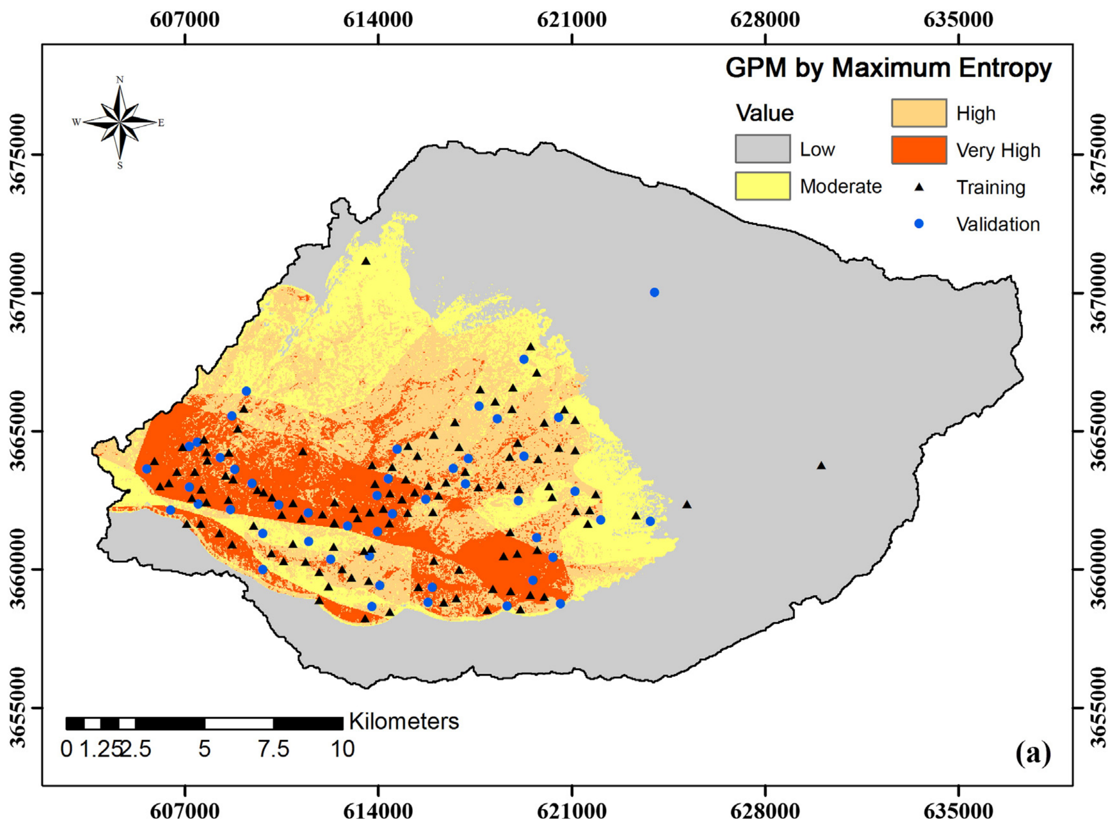

Fig. 9. Groundwater potential map produced by ME model.

other hand, the prediction-rate curve used the validation groundwater well locations (i.e. 30% groundwater well samples) which determined how well the model and conditioning factors anticipates the groundwater occurrence (Pradhan, 2013).

For quantitative comparison of RF and ME models, the areas under the prediction-rate curves were considered. As shown in Figs. 10b and 11b, the AUC for the prediction-rate curve of the GPMs produced by RF and ME models were 83.1% and 87.7%, respectively. Therefore, the ME model (AUC = 87.7%) performs better than RF model (AUC = 83.1%). In comparison with AUC classification in Yesilnacar (2005), it can be seen that both models (all AUC > 80%) applied in this study showed reasonably very good accuracy in spatial prediction of groundwater potential. Based on the attained accuracies, it is obvious that the RF and ME models can be applied as efficient machine learning models in groundwater potential mapping.

The RF and ME are useful to model natural phenomena (e.g. groundwater potentiality and groundwater occurrence) with nonlinear relationships. These machine learning models does not need prior elimination of outliers or data transformation, statistical assumptions, and can fit complex nonlinear relationships between groundwater conditioning factors and groundwater potentiality and automatically analyze interaction effects between groundwater conditioning factors

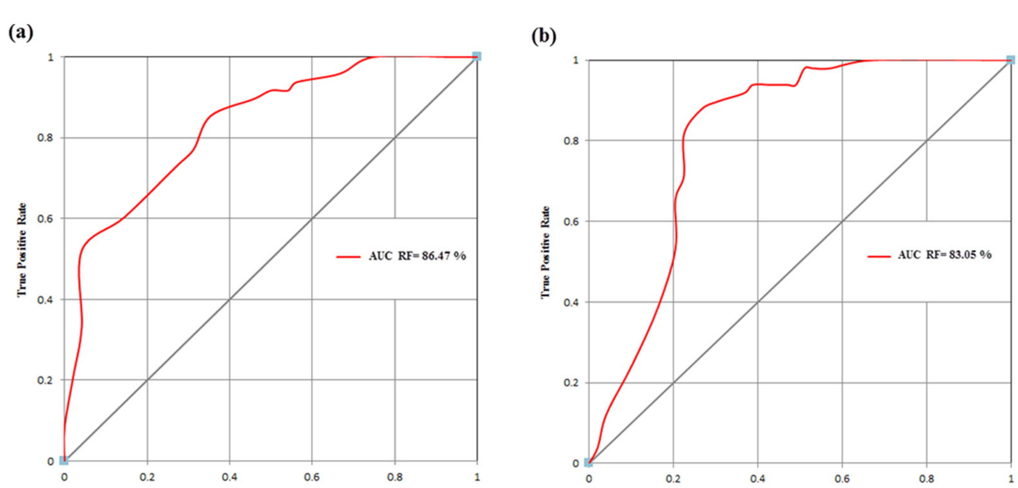

Fig. 10. ROC curve: (a) success rate (b) prediction rate for RF model.

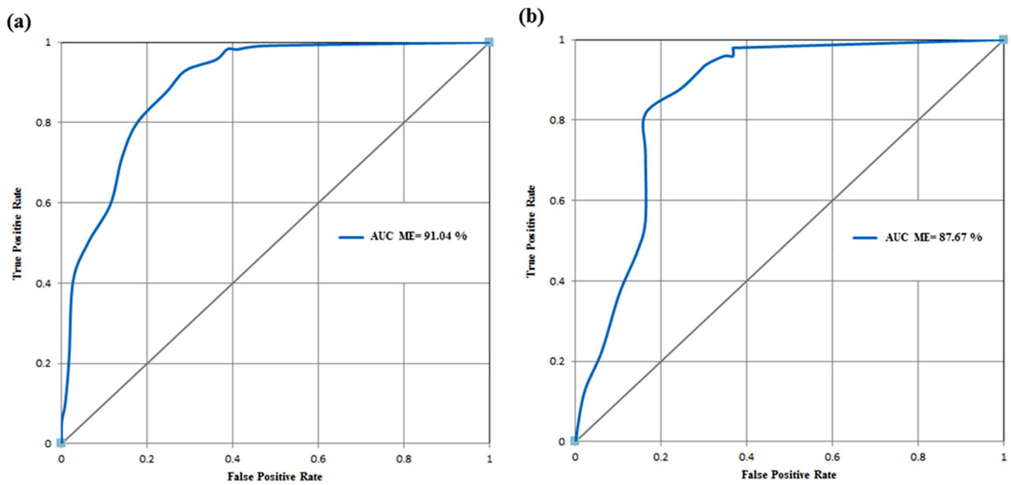

Fig. 11. ROC curve: (a) success rate (b) prediction rate for ME model.

(i.e. predictors). It is important to notice that the parameter *mtry* in the RF model was optimized via the internal RF function TuneRF which needs to be considered in the analysis.

4. Conclusion

Groundwater potentiality analysis is one of the most popular areas of research, especially in arid and semi-arid regions. Various approaches have been used for this purpose by numerous researchers. This study aimed to evaluate the applicability of random forest and maximum entropy models, which have been used widely for environmental and ecological modeling, but which have not been investigated for groundwater potential mapping. The current study investigated the potential application of RF and ME models in detection and prediction of spatial distribution of potential locations for groundwater exploration in Mehran Region, Iran. To produce GPM, the first step was the selection and preparation of the groundwater conditioning factor data sets (i.e. altitude, slope percent, slope aspect, plan curvature, drainage density, distance from rivers, TWI, landuse, lithology, and soil texture) which affect the groundwater potentiality. Then, the groundwater data (with a yield of ≥11 m^3/h) were randomly split into a training dataset 70% (114 groundwater well locations) for training the model and the remaining 30% (49 groundwater well locations) was used for validation purpose. Using the mentioned conditioning factors, GPMs were produced using RF and ME models, and the results were plotted in GIS environment. The validation results indicated that the ME model (AUC = 87.7%) performs better than RF model (AUC = 83.1%). Although several groundwater conditioning factors have been continuously applied in the literature, our study provides a quantitative evaluation of the effect of variable variations on model outputs through a sensitivity analysis to assess the factor contribution and uncertainty analysis. The sensitivity analysis indicated that the GPM is most sensitive to altitude, lithology, drainage density, and landuse with percent of relative decrease (PRD) of AUC values of 11, 6.46, 5.89, and 5.32, respectively. Certainly, this study did not consider all the uncertainty sources, but current study is pioneer to apply the RF and ME models in groundwater potentiality modeling, and therefore further studies is needed to reduce their uncertainty. It is shown that, the ME model showed better predictive performance than the RF model. Furthermore, the applied models provided accurate and cost effective results. Unlike the other machine learning algorithms such as artificial neural networks (ANNs), the random forest and maximum entropy models can provide useful information for interpretations. For example, factor contribution analysis, and response curves, determined that the most important conditioning factors are altitude, lithology, landuse, and drainage density. However, one of the drawbacks of RF model is related to the required time for the analysis. Moreover, two parameters (i.e. n_{tree} and m_{try}) should be assessed in order to find the optimum values for the modeling. The results obtained in this study can be useful for comprehensive evaluation of groundwater exploration development. However, in order to have reliable judgment about the efficiency of the RF and ME models in groundwater potentiality mapping, the models need to be tested in other areas.

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