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Prediction of water pollution sources using artificial neural networks in the study areas of Sivas, Karabük and Bartın (Turkey)

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Abstract The determination of the rock types from which the water is recharged/discharged is an essential component of hydrochemical, hydrogeological and water pollution studies. Especially, detection of sources of groundwater contamination is very important in terms of human health and other living organism. This study aims at prediction of water pollution sources using artificial neural networks (ANNs) in Sivas, Karabük and Bartın areas of Turkey, which have different types of rocks, agricultural activity and mining activity. In this study, a model based on ANNs was developed for forecast to the water discharging from different types of rocks and the water pollution sources in the study areas. Back propagation and Bee Algorithm (BA) were used in ANN training. For achieving the aim of the study, 14 hydrochemical data set were used. The best ANN classification of water discharging from different type of rocks was accomplished with 80 % accuracy using BA. These results indicate that the researches that are similar to this study can provide quite convenience for the assessment of groundwater pollution sources when applied on a large and regional scale.

Keywords Hydrogeochemistry · Water contamination · Artificial neural networks (ANNs) · Bee algorithm · Turkey

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Introduction

The artificial neural networks (ANNs) are a technique for the human brain's problem-solving process (Kuo et al. 2004) and were inspired by biological neuron processing to perform brain-like computation through simple artificial neurons massively connected to identify the relationship between inputs and outputs of a system (Chang et al. 2010). ANNs are a highly interconnected network of many simple processors. These simple processors, named artificial neurons, are organized into an input layer, a hidden layer (or layers) and an output layer. The neurons are connected by their weights. The input layer takes a pattern of stimulation from the outside world and passes through the pattern to the hidden layer(s) where it is processed. Finally, an output pattern is generated and presented by the output layer (Zhang and Stanley 1997). The advantages of applying ANNs to water quality simulation are: (1) no physics-based algorithm is required to build the model; therefore, the modeling approach is faster and more flexible than physicsbased modeling approaches in most cases; (2) ANNs can handle non-linear relationship easily and properly; and (3) the expertise and user experiences could be incorporated easily into the model structure (Zhang and Stanley 1997; Chang et al. 2010).

Recently, ANN-based techniques are also widely used in the fields of environmental science, hydrogeology, engineering geology, etc.; Verma and Singh (2013) have predicted the water quality parameters as biological oxygen demand and chemical oxygen demand via simple field parameters like temperature, pH, etc. Tasdemir et al. (2013) used 3 different ANN model (feedforward back propagation, radial basis function-based neural network and generalized regression neural networks) for estimating slake durability index which assess the resistance of clay-bearing and weak rocks to erosion and degradation. Fu et al. (2013) used ANN-based techniques for prediction of dissolved organic carbon in a river network and evaluate the impacts of watershed characteristics. Furthermore, in the studies which are dealing with water investigation, ANNs has been widely used to forecast the precipitation and the relationships between discharge and river stage, rainfall and runoff modeling, determination of groundwater salinity and contamination, recovering the missing arsenic data and other hydrological and hydrogeochemical applications (Kuo et al. 2004; Jeong and Kim 2005; Kumar et al. 2006; Sahoo et al. 2006; Yesilnacar et al. 2008; Jaafar et al. 2010; Chang et al. 2010; Seyam and Mogheir 2011; Moasheri et al. 2012; Alagha et al. 2013).

The Bee Algorithm (BA) is an optimization algorithm inspired by the natural foraging behavior of honey bees (Pham et al. 2005, 2006). A colony of honey bees can extend itself over a 5 km distances and through multiple directions to exploit food sources (Seeley 1996). Collective intelligence of bee swarms is based on the information exchange between honey bees. This information includes food source location, direction and amount of nectar. Every single bee shares the information they have on a kind of stage with others. They exchange information by dancing on a stage in the hive (Von Frisch 1967; Camezine and Sneyd 1991).

The BA can be explained briefly as below (Düğenci 2007);

Pseudo Code:

- 1. Set parameter and initialize bee colony with random method
- 2. Evaluate the fitness value of each bee to represent solution
- 3. Repeat steps while stopping criteria are not met
- 4. Define neighborhood search area
- 5. Send bees to selected area (more bees for area where fitness value is high)
- 6. Select the fittest bees
- 7. Send new bees for random search and evaluate the fitness
- 8. End While

The algorithm requires a number of parameters to be set, namely: number of scout bees (n), number of sites selected out of n visited sites (m), number of best sites out of m selected sites (e), number of bees recruited for best e sites (nep), number of bees recruited for the other (m-e)selected sites (nsp), initial size of patches (ngh), which includes site and its neighborhood and stopping criterion. The algorithm starts with the n scout bees being placed randomly in the search space. The fitnesses of the sites visited by the scout bees are evaluated in step 2.

In step 4, bees that have the highest fitnesses are chosen as "selected bees" and sites visited by them are chosen to search the neighborhood. Then, in steps 5 and 6, the algorithm conducts searches in the neighborhood of the selected sites, assigning more bees to search near to the best e sites. The bees can be chosen directly according to the fitnesses associated with the sites they are visiting. Alternatively, the fitness values are used to determine the probability of the bees being selected. Searches in the neighborhood of the best e sites which represent more promising solutions are made more detailed by recruiting more bees to follow them than the other selected bees. Together with scouting, this differential recruitment is a key operation of the BA. However, in step 6, for each patch only the bee with the highest fitness will be selected to form the next bee population. In nature, there is no such a restriction. This restriction is introduced here to reduce the number of points to be explored. In step 7, the remaining bees in the population are assigned randomly around the search space scouting for new potential solutions. These steps are repeated until a stopping criterion is met. At the end of each iteration, the colony will have two parts to its new population-representatives from each selected patch and other scout bees assigned to conduct random searches (Düğenci 2007).

In this study, there are five separate study regions of Turkey (Fig. 1). The first study area (Tecer Mountain) is located in the Central Anatolia Region, east of Ulas (SE of Sivas) and has a catchment area of approximately 394 km². Tecer Mountain and its vicinity have generally karstic limestone and clastic rocks (Ekemen 2001). The second study area (Yıldız River Basin) is located in the Central Anatolia Region, northwest of Sivas and its catchment area is approximately 1430 km² (Ekemen 2006). In Yıldız River Basin generally limestone, marble, travertine, volcanic and plutonic rocks and ophiolitic rocks crop out. The third study area (Eskipazar) is located 35 km southwest of Karabük province in the Eastern Black Sea Region and has a catchment area of approximately 625 km² (Keskin 2010a, b). Eskipazar study area is covered generally by flysh, limestone and clastic rocks in which agricultural activities are carried out. The fourth study area (Koyulhisar) is located in on the boundary of the East Black Sea Region and Center Anatolian Region, approximately 220 km northwest of the Sivas and has a catchment area of approximately 390 km² (Keskin and Toptas 2012). Koyulhisar study area comprises volcanic rocks and has active Pb-Zn-Cu mining. The fifth study area (Bartin) is located in the West Black Sea Region, approximately 283 km north of the province of Ankara and its catchment area is approximately 2200 km² (Keskin 2013). The rocks in the Bartin study area consists generally of very altered volcanic, clastic, carbonate rocks. Active coal mining is carried out in this area. Coal veins in region



Fig. 1 Location of the study areas and its vicinity

are located in Carboniferous clastic units, which overlain by volcanic rocks.

The geochemistry of groundwater is based on the geological setting, mine activity, agricultural activity and other human activity, etc. For example, the water discharging from carbonate rocks have highly likely to be Ca–HCO₃ facies; and the water flowing through sulfide deposits might have probably Ca–SO₄ facies. The groundwater in an area that is carried out agricultural activity might have probably NO₃ and some trace elements pollution caused by fertilizers and pesticides (Keskin 2010a). The groundwater that issue from the very altered volcanic rocks might have probably Na–HCO₃ facies due to alteration of volcanics, progressive silicate hydrolysis, precipitation of minerals and ion exchange reactions (Na exchange Ca and Mg) (Reidel et al. 2002; Vlassopoulos et al. 2009; Jeong 2001; Keskin 2013).

Geological background

The geological map of Tecer Mountain and its vicinity (1:100,000 scale) is taken from Gürsoy (1986), Gökten

(1993), İnan (1987), İnan et al. (1993) with some minor revision (Fig. 2). The basement rocks of the study area consist of Upper Jurassic-Early Cretaceous Çataldağ Limestone unconformably overlain by Upper Cretaceous Divriği Ophiolitic Melange, Maestrichtien–Thanetion Tecer Limestone, and other younger sedimentary formations. (Gürsoy 1986; Gökten 1993; İnan 1987; İnan et al. 1993).

The Yıldız River Basin study referred to previous geological studies of the Yılmaz (1982), Yağmur (1996) and Yılmaz et al. (1997) (revising some parts) in compiling a 1:100,000 scale geological map (Fig. 3). The basement rocks of the study area consist of Early Upper Cretaceous– Paleocene Akdağmadeni Lithodeme and Upper Cretaceous– Paleocene Tekelidağ Melange. These older units are cut by Maestrichtien–Paleocene Darmik volcanics and Pazarcık volcanics. Eocene, Miocene and Pliocene clastic and mixed clastic and carbonate rocks unconformably overlay all old units (Yılmaz 1982; Yağmur 1996; Yılmaz et al. 1997).

In Eskipazar study, the geological studies of Şaroğlu et al. (1995), Tokay (1973), Alan and Aksay (2002), Timur and Aksay (2002), Sevin and Aksay (2002) and Bilginer et al. (2002) were used (with revision in some parts) and a geological map of the study area was produced at a scale of



Fig. 2 Geological-hydrogeology map of the Tecer Mountain (Sivas) study area and its vicinity (The geological maps are taken from Gürsoy 1986; Gökten, 1993; İnan 1987; İnan et al. 1993 with revision)

1:100,000 (Fig. 4). This study area is located in a region where Western Pontides and Central Sakarya Zone come together along the Northern Anatolian Fault Zone (NAFZ). In the northern part of the NAFZ, the basement of the Western Pontide is made up of pre-Ordovician Bolu Granitoid. This basement is overlain unconformably by Paleozoic Mesozoic limestone and clastic rocks. These units are covered by the Eocene volcanic and sedimentary units. A subsection of the Sakarya Zone, in the south of the NAFZ, includes the Callovian-Aptian limestone. This unit is conformably overlain by the Albian-Maestrichtien sandstone and limestone, the Upper Miocene basalt, the Pliocene clastic (Örencik Formation), travertine and alluvium (Saroğlu et al. 1995; Tokay 1973; Alan and Aksay 2002; Timur and Aksay 2002; Sevin and Aksay 2002; Bilginer et al. 2002).

In Koyulhisar study, previous geological studies by MTA (2009), Altun et al. (1994), Uysal et al. (1995) and Gökçe and Özgüneylioğlu (1988) (with revision in some parts) were utilized and a geological map of the study area was produced at a scale of 1:100,000 (Fig. 5). The oldest rock unit of the study area is made up of Upper Cretaceous volcanics which has Pb–Zn–Cu ore deposits. This unit is overlain by Upper Cretaceous–Paleocene plutonics. These units are covered by Eocene plutonics, volcanics and sed-imentary rocks. All older rock units in the Koyulhisar area are overlain by Pliocene volcanics and Quaternary

alluvium (MTA 2009; Altun et al. 1994; Uysal et al. 1995; Gökçe and Özgüneylioğlu 1988) (Fig. 5).

For Bartin study, previous geological studies by Akbaş et al. (2002), Gedik and Aksay (2002), Alan and Aksay (2002) and Timur and Aksay (2002) (with revision in some parts) were used to produce a geological map (1:100,000 scale) of the study area (Fig. 6). The basement rocks of the region consist of Precambrian metamorphics unconformably overlain by sedimentary Devonian rocks. These units are overlain by Devonian and Carboniferous clastic and carbonate rocks. Coal veins are located among the Carboniferous clastic rocks. These units are covered unconformably by Permo-Triassic terrestrial clastics and Triassic lacustrine clastics and carbonates that are transitional with each other. These older rock units are overlain by Jurassic and Cretaceous clastic, carbonate rocks and occasional volcano-sedimentary and volcanic rocks, in turn overlain unconformably by Eocene volcanic, volcano-sedimentary and clastic rocks. The uppermost lithology unit comprises Quaternary alluvium (Akbaş et al. 2002; Gedik and Aksay 2002, Alan and Aksay 2002; Timur and Aksay 2002) (Fig. 6).

Materials and methods

The study was conducted within a time period from 2000 to 2010 at five different regions. Data were collected from



Fig. 3 Geological-hydrogeology map of the Yıldız River Basin (Sivas) study area and its vicinity (The geological maps are taken from Yılmaz 1982; Yağmur 1996; Yılmaz et al. 1997 with revision)



Fig. 4 Geological–hydrogeology map of the Eskipazar (Karabük) study area and its vicinity (The geological maps are taken from Şaroğlu et al. 1995; Tokay 1973; Alan and Aksay 2002; Timur and Aksay 2002; Sevin and Aksay 2002; Bilginer et al. 2002 with revision)



Fig. 5 Geological-hydrogeology map of the Koyulhisar (Sivas) study area and its vicinity (The geological maps are taken from MTA 2009; Altun et al. 1994; Uysal et al. 1995; Gökçe and Özgüneylioğlu 1988 with revision)

137 springs and 24 wells in the five different study areas (But some waters which are geothermal origin, the number of group of less than 5, and has extreme values (4 water) in term of chemical composition were removed and total 129 springs and wells were analyzed in ANN model). Electrical conductivity (EC), pH, total dissolved solids (TDS) and temperature (T) measurements were performed in situ using portable electrometers. Water samples were taken into polyethylene bottles for chemical analysis. The pH meter was calibrated using two buffers (pH = 4 and 7) and recalibrated periodically in the field to reduce instrumental drift. For trace element analysis, samples were filtered through a 0.45-µm membrane and then acidified to pH < 2.0 with nitric acid (HNO₃). Water samples were stored in a refrigerator prior to analysis. Major anion and cation analyses of water samples were carried out using a high-performance ion chromatography system (HPIC) at the Water Chemistry Laboratory of Hacettepe University (Turkey), and ion chromatography (Dionex-1000) system at Department of Geological Engineering of Cumhuriyet University (Turkey). HCO₃-CO₃ ions were analyzed using the standard titration method at Water Chemistry

Laboratory, Cumhuriyet University (Turkey). Trace elements were measured using inductively coupled plasmamass spectrometry, ICP-MS, at Hacettepe University, and at the AcmeLabs Laboratory (Canada).

This research is based on the water chemistry information from 129 groundwater samples for ANN analyses. The information gathered by means of field measurements and laboratory analyses includes Na, K, Ca, Mg, CO₃, HCO₃, Cl, SO₄, Fe, Mn, Al, pH, EC and NO₃. In the first step, data were being normalized and imported into the ANN software written by Düğenci (2007) in the Java language for the estimation of 6 output parameter using 8 input parameter of a treatment plant. Software was developed as Java Swing application using Oracle J Developer Suite development tool. In this article, multilayer perceptron (MLP) model with 14 input neuron and with one hidden layer (with 5 neurons) was used. 99 and 30 data were analyzed for training and testing of the model, respectively. Finally, prediction of water contamination sources and the waters discharging from different rock types with 1 output neuron classifier was carried out. Back propagation (BP) and BA are used in ANN training.



Fig. 6 Geological-hydrogeology map of the Bartin study area and its vicinity (The geological maps are taken from Akbaş et al. 2002; Gedik and Aksay 2002; Alan and Aksay 2002; Timur and Aksay 2002 with revision)

Hydrogeology and water contamination

The main aquifer in the Tecer Mountain study area is Tecer Limestone. The limestone is densely fractured, jointed and karstified. There are many springs discharging from this unit (Fig. 2; Table 1) (Ekemen 2001). The units that determine the main aquifer characteristics in the Yıldız River Basin are generally carbonate rocks (Üçtepe Limestone, Akdağmadeni Lithodeme consisting of very fractured marble and travertine) and clastic rocks (İncesu Formation). There are many springs discharging from these aquifers (Fig. 3; Table 2) (Ekemen 2006).

The units indicating primary aquifer characteristics in the Eskipazar study area are Abant Formation consisting of layers of limestone and flysh; Soğukçam Formation comprising intensive fractured crystallized limestones and Örencik Formation consisting of limestone and slightly cemented conglomerate, sandstone, mudstone, siltstone and claystone (Fig. 4) (Keskin 2010b). In the Eskipazar study area, nitrate pollution (NO₃) is observed in the water discharging from the Örencik Formation where agricultural activities are carried out. NO₃ pollution is highest in the wells drilled in the clastic levels of the formation. NO₃ concentrations in these wells generally exceed/or are close to the limit values of 50 mg/l given in Turkish Regulation Concerning Water Intended for Human Consumption

(Republic of Turkey Ministry of Health 2005) and the WHO (2006) regulations. NO₃ concentrations are at low levels in springs of the formation discharging from mainly limestone layers (Table 3; Fig. 4). The waters are used for drinking, domestic and irrigational purposes. (Keskin 2010a, b).

The aquifers in the Koyulhisar study area generally consist of volcanic and plutonic rocks. Upper Cretaceous volcanics consist of intensively fractured, altered, basalt, andesite, dacite and volcanoclastic rocks. There are a lot of springs discharging from these aquifers (Fig. 5). The groundwater samples discharging from Upper Cretaceous volcanics containing ore deposits generally have high acidity due to oxidation of pyrite. The pH values of these waters range between 3.3 and 4.8 and these values are below the lower limit values (6.5) in the Turkish standards. In addition, trace element pollutants (Al, Fe and Mn) are observed especially in these spring, and generally exceed the upper limits specified for these elements in the Turkish standards and World Health Organization regulations. Spring water discharging from other geological formations is generally alkaline and close to alkaline (Table 4) (Keskin and Toptas 2012).

The main aquifers in the Bartın study area are İnaltı Formation consisting of karstic limestone; Ulus Formation comprising sandstone and conglomerate; and Yemişliçay Formation which consist of rocks are volcanogenic sandstone, aglomera, andesite, basalt and limestone (Fig. 6).

Number	Date	pН	EC	Na	К	Ca	Mg	CO ₃	HCO ₃	Cl	SO_4	Fe	Mn	Al	NO
TK-2	03.07.2000	7.85	300	5.29	0.39	40	8.512	0	122	9.23	21.6	0.00002	0.000005	(-)	(-)
TK-3	05.07.2000	7.36	490	5.52	0.39	60	24.32	0	210.45	3.55	52.8	0.00002	0.000005	(-)	(-)
TK-4	05.07.2000	8.34	357	30.59	2.34	20	13.376	0	146.4	4.97	31.68	0.00002	0.000005	(-)	(-)
TK-6	05.07.2000	7.52	420	7.59	0.39	48	18.24	0	137.25	11.36	54.72	0.00002	0.000005	(-)	(-)
TK-7	06.07.2000	7.16	535	10.12	0.39	58	19.456	0	213.5	19.88	21.6	0.00002	0.000005	(-)	(-)
TK-9	06.07.2000	7.62	530	1.84	0.39	60	27.968	0	195.2	2.84	67.2	0.00002	0.000005	(-)	(-)
TK-10	06.07.2000	7.7	300	0.69	0.39	34	17.024	0	125.05	3.55	35.04	0.00002	0.000005	(-)	(-)
TK-11	06.07.2000	7.84	375	2.3	0	58	9.728	0	161.65	12.07	37.92	0.00002	0.000005	(-)	(-)
TK-12	07.07.2000	7.85	250	0.69	0	42	6.08	0	140.3	2.84	5.76	0.00013	0.000005	(-)	(-)
TK-13	07.07.2000	7.92	338	2.07	0.39	44	10.944	0	155.55	2.84	24	0.00002	0.000005	(-)	(-)
TK-14	07.07.2000	7.9	255	2.3	0	34	9.728	12	106.75	4.97	14.88	0.00002	0.000005	(-)	(-)
TK-15	07.07.2000	7.64	230	0.69	0	32	7.296	0	109.8	2.13	6.24	0.00002	0.000005	(-)	(-)
TK-19	10.07.2000	7.51	350	1.38	0.39	46	7.296	0	134.2	0.71	12.96	0.00002	0.000005	(-)	(-)
TK-21	11.07.2000	7.29	254	1.38	0	36	6.08	0	106.75	2.13	12.48	0.00002	0.000005	(-)	(-)
TK-23	11.07.2000	8.45	225	1.38	0.78	44	0.9728	6	88.45	4.97	12	0.00002	0.000005	(-)	(-)
TK-24	11.07.2000	7.92	395	0.69	0	56	4.864	0	155.55	2.13	9.12	0.00002	0.000005	(-)	(-)
TK-25	12.07.2000	7.66	268	0.46	0	48	4.864	0	146.4	1.42	3.36	0.00002	0.000005	(-)	(-)
TK-26	12.07.2000	7.87	288	0.69	0.39	52	2.432	0	140.3	1.42	12	0.00002	0.000005	(-)	(-)
TK-27	12.07.2000	8.1	313	0.69	0	56	1.216	0	146.4	1.42	24	0.00002	0.000005	(-)	(-)
TK-29	13.07.2000	8.15	268	0.92	0	34	3.648	0	109.8	1.42	6.24	0.00002	0.000005	(-)	(-)
TK-31	13.07.2000	8.06	215	0	0	36	4.864	0	103.7	2.13	12	0.00002	0.000005	(-)	(-)
TK-32	13.07.2000	7.94	380	1.38	0.39	60	3.648	0	140.3	1.775	48	0.00002	0.000005	(-)	(-)

Table 1 Field measurement data and chemical analysis results [mg/l (EC: μ S/cm)] of the groundwaters in the Tecer Mountain study area (Sivas)(Ekemen 2001)

Table 2 Field measurement data and chemical analysis results $[mg/l (EC:\mu S/cm)]$ of the groundwaters in the Yıldız River Basin (Sivas) (Ekemen 2006)

Number	Date	pН	EC	Na	K	Ca	Mg	CO ₃	HCO ₃	Cl	SO_4	Fe	Mn	Al	NO ₃
YK-1	14.07.2003	8.69	298	3.22	2.73	35	10.336	6	134.2	3.905	11.52	0.00002	0.000005	0.0005	(-)
YK-10	17.07.2003	7.7	546	4.6	0	60	26.752	0	286.7	2.13	15.84	0.00002	0.0028	0.0005	(-)
YK-11	17.07.2003	7.9	410	9.43	0.78	63	9.728	0	237.9	2.84	8.64	0.00002	0.000005	0.0005	(-)
YK-22	19.07.2003	7.24	802	7.59	1.17	123	13.376	0	402.6	7.81	14.4	0.00002	0.000005	0.0005	(-)
YK-24	19.07.2003	6.95	783	6.9	1.17	131	11.552	0	417.85	8.52	13.44	0.00002	0.000005	0.0005	(-)
YK-26	21.07.2003	7.62	556	7.82	0.78	83	12.768	0	298.9	4.97	9.6	0.00193	0.00596	0.0005	(-)
YK-32	21.07.2003	7.15	1050	14.95	1.95	166	19.456	0	555.1	10.65	28.8	0.00002	0.000005	0.0005	(-)
YK-33	21.07.2003	7.13	1017	12.42	1.95	113	43.776	0	549	12.425	25.44	0.00002	0.000005	0.0005	(-)
YK-35	21.07.2003	7.24	1100	14.72	1.95	160	37.696	0	622.2	7.1	27.84	0.00002	0.000005	0.0005	(-)
YK-52	28.07.2003	7.81	376	11.96	0.39	49	10.336	0	201.3	1.42	8.64	0.00002	0.000005	0.0005	(-)
YK-54	28.07.2003	7.81	247	0.92	0	47	0.608	0	131.15	1.775	4.8	0.00002	0.000005	0.0005	(-)
YK-57	28.07.2003	7.37	360	2.76	1.17	66	1.216	0	183	1.775	7.2	0.00002	0.000005	0.0005	(-)
YK-71	31.07.2003	7.95	277	1.84	0.39	52	1.824	0	158.6	1.065	0.48	0.00002	0.000005	0.0005	(-)
YK-76	01.08.2003	7.6	318	0.46	0	48	7.296	0	176.9	0.71	1.92	0.00002	0.000005	0.0005	(-)
YK-83	04.08.2003	7.9	340	3.22	0.39	40	8.512	0	213.5	0.71	0	0.00048	0.0049	0.0005	(-)
YK-86	04.08.2003	7.46	426	5.06	0.39	60	6.688	0	225.7	1.775	2.88	0.00002	0.000005	0.0005	(-)

Volcanic areas have undergone intensive alteration. Coal layers containing regions are overlain by Upper Cretaceous volcanics. In this area, pH values of waters discharging from Yemişliçay Formation consisting of volcanics are between 6.38 and 9.13. Springs have lower pH (6.38–7.03) values while well have higher pH (generally 7.54–9.13) values (Table 5). It is thought that the reason for having high pH values of wells discharging from this formation is mostly

Table 3 Field measurement data and chemical analysis results [mg/l (EC:µS/cm)] of the groundwaters in the Eskipazar study area (Karabük) (Keskin 2010a, b)

Number	Date	pН	EC	Na	Κ	Ca	Mg	CO ₃	HCO ₃	Cl	SO_4	Fe	Mn	Al	NO ₃
EK-1	23.07.2007	7.09	418	1.38	1.17	4.8	50.8288	0	256.2	1.42	1.92	0.0706	0.00514	0.1113	1.24
EK-2	23.07.2007	7.13	356	1.15	1.56	10.2	26.6304	0	164.7	1.42	1.92	0.0911	0.00583	0.1158	0.31
EK-5	23.07.2007	7.1	422	2.99	1.17	11	43.2896	0	244	0.71	2.4	0.2231	0.02989	0.1241	0.31
EK-6	23.07.2007	7.22	404	2.07	1.17	14.2	41.4656	0	234.85	0.355	1.92	0.0882	0.0099	0.117	0.62
EK-7	24.07.2007	6.93	525	2.53	1.95	16.6	63.232	0	347.7	1.42	3.36	0.08	0.00554	0.1188	1.24
EK-8	24.07.2007	7.06	507	3.45	3.12	7	42.1952	0	213.5	2.485	6.24	0.0786	0.00512	0.1137	12.4
EK-9	24.07.2007	7.26	457	2.99	1.56	6.4	57.152	0	271.45	1.065	7.2	0.0609	0.00465	0.1018	0.31
EK-10	24.07.2007	7.09	506	5.52	3.12	19.6	51.3152	0	286.7	4.615	8.16	0.0867	0.00584	0.1159	11.2
EK-12	24.07.2007	7.09	554	2.3	1.56	8.4	51.1936	0	286.7	0.71	3.84	0.0758	0.00512	0.1094	0.31
EK-14	25.07.2007	7.22	440	2.07	1.17	3.6	43.168	0	204.35	0.71	2.4	0.0506	0.00454	0.0993	4.34
EK-15	25.07.2007	6.98	549	2.53	1.56	10	53.7472	0	286.7	1.065	5.28	0.0627	0.00474	0.1027	0.31
EK-17	25.07.2007	7.05	503	1.61	1.56	6	48.3968	0	265.35	0.355	2.88	0.0567	0.00465	0.0963	0.31
EK-18	25.07.2007	7.09	457	1.38	1.56	4.8	50.5856	0	259.25	0.355	1.92	0.0556	0.00454	0.0934	0.31
EK-19	25.07.2007	6.75	711	17.94	2.73	32.2	56.0576	0	390.4	6.035	20.64	0.0547	0.00432	0.0957	3.1
EK-23	26.07.2007	7.92	359	1.15	1.56	15.8	31.3728	0	198.25	0.71	5.28	0.0772	0.00503	0.0993	0.31
EK-24	26.07.2007	6.99	573	1.84	1.56	9	72.352	0	362.95	1.775	4.8	0.07	0.00473	0.0971	0.31
EK-25	26.07.2007	7.04	506	1.38	1.56	5.4	46.6944	0	247.05	0.71	5.76	0.0497	0.00425	0.0969	0.62
EK-26	26.07.2007	7.11	426	1.15	1.56	4.4	47.3024	0	240.95	0.71	7.68	0.0564	0.00424	0.0981	1.86
EK-30	27.07.2007	7.09	800	69	7.02	69	42.8032	0	430.05	11.005	73.44	0.048	0.00425	0.0946	3.72
EK-31	27.07.2007	7.12	507	16.1	3.12	23.6	42.0736	0	292.8	5.68	9.12	0.0595	0.00454	0.0958	1.24
EK-32	27.07.2007	7.09	491	13.11	2.73	19.6	26.752	0	231.8	3.905	6.72	0.7517	0.00947	0.0971	0.62
EK-33	27.07.2007	6.75	794	22.77	3.12	42.6	53.0176	0	393.45	8.52	36.48	0.0545	0.00426	0.0962	3.72
EK-35	28.07.2007	7.19	462	7.36	2.34	24.6	38.1824	0	256.2	3.195	14.4	0.0878	0.00506	0.0954	1.24
EK-36	20.08.2007	7.42	523	13.57	3.12	19	48.8832	0	271.45	10.295	11.52	0.0457	0.00434	0.0928	37.8
EK-37	20.08.2007	7.04	658	20.24	0	26.2	60.8	0	353.8	9.23	16.32	(-)	(-)	(-)	21.1
EK-38	28.07.2007	7.15	790	93.61	3.12	40.8	41.2224	0	451.4	24.495	29.28	0.0657	0.00044	0.0153	34.7
EK-40	16.10.2007	7.16	1130	63.48	3.9	99.6	47.7888	0	405.65	47.215	37.92	0.176	0.00016	0.1308	123
EK-41	20.04.2008	6.99	566	20.24	3.9	33.4	50.8288	0	298.9	10.295	17.76	0.0075	(-)	0.0143	1.86
EK-43	06.08.2008	7.2	930	100.05	2.34	40.2	32.224	0	430.05	26.27	31.68	(-)	(-)	(-)	24.2
EK-44	11.08.2008	6.96	630	19.55	0.78	21.2	58.8544	0	311.1	9.94	14.88	(-)	(-)	(-)	27.3
EK-45	11.08.2008	7.21	693	38.18	0.78	21.6	45.7216	0	308.05	16.685	23.04	(-)	(-)	(-)	32.2
EK-46	06.08.2008	7.34	1006	78.43	3.12	25.6	51.68	0	366	56.445	32.64	(-)	0.01014	0.1348	130

progressive alteration of silicates (e.g., basalts) (Reidel et al. 2002; Vlassopoulos et al. 2009; Keskin 2013). Trace element pollutants (Al, Fe and Mn) are observed in water discharging from the Yemişliçay Formation and clastics rocks containing coal veins and generally exceed the upper limit specified in the Turkish standards and World Health Organization regulations (Keskin 2013).

Training ANN with Bee Algorithm

The ANN can be evaluated as minimization of an error function in ANN training. Error function calculates the difference between the output of the training set and desired (ideally) output. Training process is performed by giving to ANN of randomly selected samples in each case. While the training set samples are being shown to network, the sums of square of the difference between desired and obtained values is determined simultaneously. As a result of this process, the total error value generated from the error function of net value for the weight values is determined (Karaboga and Öztürk 2009 ; Ghassan and Aman 2011).

In terms of BA, each bee represents an ANN weight vector. The purpose of the algorithm is to find the bee that had weight vector producing the lowest error value. The ANN model with single hidden layer and bias is given below;

Number	Date	pН	EC	Na	K	Ca	Mg	CO ₃	HCO ₃	Cl	SO_4	Fe	Mn	Al	NO ₃
KK-1	27.07.2009	4.8	53	1.61	1.17	3.6	0.9728	0	12.2	0.71	13.44	0.021	0.02261	0.600	0.62
KK-2	27.07.2009	3.84	151	1.38	1.95	3.6	0.7296	0	9.15	0.71	32.16	0.776	0.00634	2.700	0.31
KK-5	28.07.2009	6.44	33	1.61	0.78	4	0.3648	0	15.25	0.355	1.92	0.021	0.00237	0.041	6.2
KK-6	28.07.2009	7.69	66	1.61	0.78	6.6	1.216	0	24.4	0.71	2.4	0.102	0.00727	0.143	3.72
KK-7	28.07.2009	6.27	210	2.99	1.17	26.2	2.1888	0	30.5	0.71	56.64	0.144	0.01893	1.730	0.62
KK-8	28.07.2009	7.09	27	1.38	0.39	3.2	0.1216	0	12.2	0	1.92	0.005	0.00096	0.038	0.31
KK-9	29.07.2009	7.09	27	1.38	0	3	2.1888	0	15.25	0.355	1.44	0.022	0.00418	0.078	1.24
KK-10	29.07.2009	6.9	26	1.15	0.39	2.8	0.3648	0	12.2	0.355	1.44	0.015	0.00255	0.062	2.48
KK-11	29.07.2009	3.94	112	1.38	1.95	7.2	1.216	0	3.05	0.355	36.48	0.052	0.04861	2.306	0.31
KK-12	29.07.2009	3.53	211	0.92	1.95	4	1.4592	0	3.05	0.355	45.6	0.005	0.08608	3.452	0.31
KK-14	31.07.2009	6.9	88	2.99	3.51	8.8	0.7296	0	36.6	0.71	2.88	0.035	0.0023	0.127	0.62
KK-15	31.07.2009	6.9	38	2.76	1.17	2.6	0.3648	0	15.25	0	0	0.005	0.00111	0.037	1.24
KK-16	31.07.2009	7.28	45	3.45	1.56	3.4	0.4864	0	21.35	0.355	0.48	0.005	0.00231	0.070	2.48
KK-17	31.07.2009	6.93	37	2.76	0.39	2.6	0.4864	0	15.25	0.355	2.88	0.02	0.0042	0.078	2.48
KK-19	31.07.2009	3.65	248	2.53	1.56	11.6	2.1888	0	6.1	0.355	75.84	0.084	0.06623	5.700	0.31
KK-20	01.08.2009	6.63	103	3.91	1.17	10.4	1.4592	0	39.65	0.71	2.88	0.005	0.00201	0.075	5.58
KK-21	01.08.2009	6.42	47	2.76	1.95	3.4	0.608	0	21.35	0.355	0.96	0.005	0.0011	0.055	1.24
KK-22	01.08.2009	7.96	39	3.68	1.56	2	0.4864	0	15.25	0.355	0	0.005	0.00095	0.058	0.62
KK-23	01.08.2009	6.8	49	2.76	1.56	3.4	0.7296	0	24.4	0.355	0.96	0.011	0.00153	0.080	1.24
KK-24	01.08.2009	6.84	33	2.07	1.17	2.6	0.2432	0	15.25	0	0.96	0.005	0.00082	0.046	1.24
KK-25	01.07.2009	6.97	113	6.44	0.39	10.8	2.1888	0	54.9	0.355	1.92	0.005	0.00178	0.066	0.62
KK-26	01.07.2009	7.57	73	6.21	0	5.6	0.9728	0	30.5	0.355	0.96	0.005	0.00148	0.070	1.86
KK-27	01.07.2009	7.31	88	6.21	0.39	7.6	1.3376	0	42.7	0.355	0.96	0.005	0.00054	0.032	1.24
KK-29	02.08.2009	7.3	138	5.75	2.73	15.8	2.0672	0	67.1	0.355	1.92	0.005	0.00157	0.085	0.62
KK-31	27.07.2009	3.6	272	1.61	1.17	3	2.0672	0	9.15	0.71	66.24	0.03	0.08976	5.462	0.31
Ministry Health 2005 ^a		6.5–9.5	2500	200							250	0.2	0.05	0.2	50
WHO 2006													0.4	0.2	50

Table 4 Field measurement data and chemical analysis results [mg/l (EC:µS/cm)] of the groundwaters in the Koyulhisar study area (Sivas) (Keskin and Toptaş 2012)

^a Republic of Turkey Ministry of Health (2005)

NG The number of input layer processor

NA The number of hidden layer processor

NC The number of output layer processor

We calculate the total weight which is represented by bee as follows. Firstly, we find the number of connections input to hidden including bias weights and hidden to output. Then, we add the number of weights between hidden plus bias and output.

The number of weight between input and hidden layer $= (NG + 1) \times N$

The number of weight between hidden and output layer = $(NA + 1) \times NC$

Total weight = $(NG + 1) \times NA + (NA + 1) \times NC$

The purpose of this study is to establish the structure represented by the total weight value, which formulated above, using the Genetic Algorithm (GA) and BA rather than BP for the determination of the weight value of ANN. Each bee in BA represents the value in the total number of weight.

There are the trial and error method and the half of the total input and output data number method, etc., for determining the number of hidden layer neuron. The trial and error method is used most commonly. The trials with 3–10, the number of hidden layer neurons were conducted in this study, and the hidden layer providing the best results is determined as 5.

For example, if we prefer an ANN model which have 14 input neurons, 5 hidden layer neurons and one output neuron with bias; we calculate the total weight as 81;

Total weight = $(14 + 1) \times 5 + (5 + 1) \times 1 = 81$

A bee will represent the 81 weight value of ANN. In other word, 100 bee colony represents 100 different ANN

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Table 5 Field measurement data and chemical analysis results [mg/l (EC:µS/cm)] of the groundwaters in the Bartin study area (Sivas) (Keskin 2013)

Number	Date	pН	EC	Na	Κ	Ca	Mg	CO ₃	HCO ₃	Cl	SO_4	Fe	Mn	Al	NO ₃
BK-1	22.06.2010	6.85	742	8.97	0.78	107.8	1.824	0	355.02	6.745	12.48	0.005	0.0105	0.035	3.72
BK-4	22.06.2010	7.06	457	1.61	0.39	85	3.7696	0	254.98	1.42	2.88	0.005	0.00101	0.014	0.62
BK-5	22.06.2010	7.51	631	5.52	1.17	86.6	6.5664	0	308.05	2.13	16.32	0.011	0.00199	0.05	0.25
BK-6	22.06.2010	7.11	439	1.61	0.39	63	7.0528	0	236.68	1.065	2.4	0.013	0.00277	0.034	0.62
BK-7	22.06.2010	7.83	445	1.61	0.39	73	8.9984	0	254.98	1.42	2.88	0.005	0.00733	0.031	0.62
BK-8	22.06.2010	6.88	847	7.82	3.9	125.4	13.4976	0	398.33	8.52	13.92	0.005	0.00127	0.012	10.5
BK-9	22.06.2010	7.21	504	2.07	0.39	71.8	18.4832	0	301.34	1.42	4.8	0.005	0.00127	0.014	0.62
BK-10	22.06.2010	7.65	553	2.07	0.78	65.6	26.2656	0	316.59	1.775	6.72	0.011	0.00312	0.026	0.62
BK-11	23.06.2010	6.89	791	8.51	5.85	132.2	7.296	0	391.62	7.455	15.84	0.005	0.00149	0.014	14.3
BK-13	23.06.2010	7.62	662	4.37	0.78	92.8	4.4992	0	286.09	1.42	2.4	0.019	0.00272	0.075	0.19
BK-14	23.06.2010	7.49	619	14.95	1.95	82.8	10.8224	0	305	2.485	16.32	0.147	0.013	0.131	0.31
BK-17	23.06.2010	6.84	638	7.13	1.56	89	11.6736	0	317.2	2.485	15.84	0.045	0.001	0.037	0.31
BK-18	23.06.2010	6.96	617	7.13	1.56	78.6	11.6736	0	279.99	2.84	15.36	0.005	0.00384	0.018	0.62
BK-21	24.06.2010	7.03	910	5.06	1.56	117	22.1312	0	432.49	6.035	14.4	0.438	0.231	0.761	1.24
BK-23	24.06.2010	7.1	181	9.2	1.17	17.6	4.0128	0	84.18	6.745	1.92	0.082	0.00468	0.031	0.31
BK-24	24.06.2010	8.45	720	137.31	0.78	10.2	0.8512	15.3	323.91	3.905	15.84	0.022	0.00902	0.019	0.31
BK-25	24.06.2010	6.82	700	8.51	1.95	106.4	4.256	0	341.6	4.615	6.24	0.005	0.00216	0.014	1.86
BK-27	24.06.2010	8.51	378	65.09	0.78	10.4	0.8512	24.6	146.4	3.195	3.36	0.068	0.02	0.048	0.31
BK-28	24.06.2010	7.15	400	21.16	1.95	48.4	6.3232	0	214.72	4.97	1.92	0.005	0.00544	0.022	0.19
BK-29	24.06.2010	7.03	154	11.04	1.95	17.8	2.6752	0	80.52	4.26	2.4	0.237	0.019	0.136	0.62
BK-31	25.06.2010	6.38	82.2	7.13	1.56	5.6	0.9728	0	28.06	4.97	2.4	0.005	0.0019	0.022	0.19
BK-32	25.06.2010	6.79	89.2	6.67	1.95	7.4	1.216	0	34.16	4.97	1.44	0.475	0.02	0.104	0.62
BK-34	25.06.2010	7.19	484	26.45	1.56	59.8	3.8912	0	223.87	6.745	14.4	0.798	0.085	0.46	0.62
BK-36	25.06.2010	6.91	490	12.65	1.56	70	4.0128	0	223.26	4.615	30.24	0.262	0.016	0.299	1.24
BK-37	25.06.2010	7.54	578	71.76	1.95	28.8	2.5536	0	273.89	5.68	9.12	0.01	0.00804	0.018	0.31
BK-38	25.06.2010	7.78	385	52.9	1.95	22	5.472	0	211.06	5.325	2.4	0.042	0.044	0.025	0.31
BK-39	25.06.2010	8.38	412	71.3	2.34	9	1.216	27.6	149.45	5.325	1.92	0.015	0.0045	0.019	0.62
BK-40	25.06.2010	8.65	414	71.99	8.58	10.4	0.8512	42.9	115.29	3.195	7.68	0.224	0.00775	0.257	0.62
BK-44	26.06.2010	7.9	390	1.15	0.39	60	9.12	0	211.67	1.065	1.44	0.015	0.00312	0.043	0.62
BK-45	26.06.2010	7.62	391	1.38	0.39	60.2	9.12	0	211.67	1.42	1.44	0.033	0.00298	0.044	0.62
BK-48	26.06.2010	7.71	399	1.84	0.78	48.6	9.9712	0	211.67	1.775	1.44	0.005	0.00171	0.029	1.24
BK-50	26.06.2010	6.91	950	17.02	2.34	144.6	4.9856	0	416.63	22.365	16.8	0.005	0.0124	0.048	11.2
BK-52	26.06.2010	6.84	930	18.17	2.34	140.8	5.1072	0	419.68	21.3	13.92	0.164	0.0104	0.029	7.44
BK-53	26.06.2010	7.04	722	8.74	1.95	105.4	6.5664	0	330.01	3.905	24.96	0.079	0.0196	0.051	2.48

weight configurations. If number of the processing element of input, hidden or output layer in the ANN change, number of weight will change.

Results and discussion

Groundwater chemical data obtained from 129 springs and wells in the Tecer Mountain, Yıldız River Basin, Eskipazar, Koyulhisar and Bartın study areas were used for the prediction of water pollution sources using ANNs. Fourteen water chemistry parameters (Na, K, Ca, Mg, CO₃, HCO₃, Cl, SO₄, Fe, Mn, Al, pH, EC and NO₃), obtained from groundwater between the years 2000 and 2010, were analyzed in ANN model.

Artificial neural network performance was measured in two ways: (1) training and (2) testing. Total 99 randomly selected water data used for training and 30 randomly selected water data used for test. Some researchers suggest that it is usually unnecessary to use more than one hidden layer in a multilayer feedforward network and varying the number of hidden nodes in the one hidden layer is usually sufficient for delivering distinct results. (Gallant 1993; El-Din and Smith 2002). In this work, one layer ANN with a

Table 6 Min, Max, Mean and Standard deviation values of BA and BP different training type, for predicting classification of water pollution sources

Training name	Min	Max	Mean	Standard deviation
BA	20	24	22.3	1.337
BA performance	0.667	0.800	0.743	0.045
BP	19	23	21.1	1.449
BP performance	0.633	0.767	0.703	0.048



Fig. 7 The ANN structure used in the study

tan-sigmoid transfer function which is most frequently preferred for the hidden layer and a linear transfer function for the output layer were used. After a number of modeling trials, the best neural network was determined to be Multilayer Perceptron Network (MLP) trained using BA with three layers: an input layer of 14 neurons, the hidden layer with 5 neurons (which is determined with the trial and error method that used most commonly), and the output layer with 1 neuron which gives the classification of water discharging from different rock types. The best ANN classification of water discharging from different type of rocks was accomplished with 80 % accuracy. Training results are provided in Table 6. Figure 7 shows the ANN structure used in the study.

The learning rate parameter could also play an important role in the convergence of the network, depending on the application and network architecture. The learning rate can be used to increase the chance of preventing the training process being trapped in a local minimum instead of a global minimum (Hamed et al. 2004; Yesilnacar et al. 2008). A larger learning rate involves a larger step. If the learning rate is too large, the algorithm becomes unstable. If the learning rate is set too small, the algorithm takes a long time to converge. In addition, the momentum allows a Table 7 Summary of one of the best in BA results

Class	Number in testing
1. Water discharging from carbonate rocks	13
2. Water discharging from mixing rocks (clastic and limestone)	7
3. Water which have nitrate pollution discharging from clastic/limestone	3
4. Alkali water (generally pH > 8) which have Al, Fe and Mn discharging from altered volcanic rocks	1
5. Acidic water which have Al, Fe and Mn discharging from volcanic rocks consisting of ore deposit	2
6. Water discharging from volcanic rocks	4

network to respond not only to the local gradient, but also to recent trends in the error surface. Without momentum, a network may get stuck in a shallow local minimum (Hagan et al. 1996; Yesilnacar et al. 2008).

In this study, the learning rate and the momentum were 0.8 and 0.2, respectively, for BP-based ANN. Furthermore, the number of scout bees (*n*-colony size), the number of sites selected out of *n* visited sites (*m*), the number of best sites out of m selected sites (*e*), the number of bees recruited for best *e* sites (nep), the number of bees recruited for the other (*m*–*e*) selected sites (nsp), the neighbor search area (ngh) and stopping criteria max iteration were 100, 20, 5, 5, 2, 0.1 and 5,000, respectively, for BA-based ANN.

In this study after experimenting with a few different methods, one of the best of them was chosen and its classes are given in Table 7. Classification of 24 water samples out of the 30 water samples were predicted correctly and classification of 6 water samples were estimated incorrectly. However, generally all incorrectly classified waters were among the ones which discharge from carbonate rocks and from the alternating (mixed) rocks. There are carbonate rocks in both the classes and it is thought that incorrect classification of the water which had complicate system in terms of recharge and discharge is normal. Furthermore, it is thought that accuracy of 80 %, which determined in this study, is also an important success in applying ANN method. Furthermore, although all classification approaches attempt to find the best possible classes, it is not generally possible due to nature of data. Data may contain unusual or outlier data where even an expert may also fail to realize the underlying reasons. In this respect, an outlier analysis may increase the accuracy rate gradually. However, since we have limited data, we did not prefer to eliminate many data with the outlier analysis. Another option to increase accuracy may be methodological enhancements (like the use of some other heuristic approaches) in possible future studies.

Conclusion

Investigations were performed on the water chemistry data from Sivas, Karabük and Bartın areas to contribute to studies aiming at classification of water contamination sources and/or of water discharging from different rock types. In this study, input factors were the water chemistry parameters consisting of Na, K, Ca, Mg, CO₃, HCO₃, Cl, SO₄, Fe, Mn, Al, pH, EC and NO₃. All these parameters were measured in the sampling area or analyzed in the laboratories, and the output factor was water discharge/ contamination sources.

There are different rock types (such as carbonate rocks, altered volcanic rocks, alternating (mixed) rocks (clastic and carbonate) and other type rocks, agricultural activities, the Pb–Zn–Cu deposits and coal mining activities in the study areas. There is NO₃ pollution in groundwater discharging from Örencik Formation in Eskipazar study area where agricultural activities are carried out. Furthermore, there are Al, Fe and, Mn element pollution in groundwater discharging from Pb–Zn–Cu mining activity area in Ko-yulhisar. There are altered volcanics and coal vein associated rocks in Bartun area.

Artificial neural network classification of water was accomplished with mean 74 % and mean 70 % accuracy using BA and BP in training, respectively. In addition, the best performance was obtained using BA with 5 neurons in hidden layer and 5,000 iterations in training and the ANN model was successfully utilized as analytical tool to determine water discharging from different rock types and water contamination sources. Furthermore, we thought that increasing the number of samples representing single aquifer, decreasing the number of samples recharging simultaneously from many rock groups, adding trace elements as Pb, Zn, Cu and As to the analysis may improve the accuracy ratio.

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