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Relationships between grain protein, Zn, Cu, Fe and Mn contents in wheat and soil and topographic attributes

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The knowledge on the relationships of protein and micronutrient concentration in wheat grain with edaphic characteristics could provide valuable information for site-specific fertilization of crops for producing grains denser in micronutrients such as iron (Fe) and zinc (Zn) in rain-fed agriculture. In this study, we used soil properties and topographic parameters in the artificial neural network (ANN) methodology as a power tool for improving models for predicting wheat grain micronutrient and protein contents in the hilly regions of western Iran. Soil and grain samples were collected from 1 m^2 plots using the stratified random method, whereas the slope positions were considered as the basis of soil sampling, at 100 selected points. The mean grain Zn, Fe, Cu (copper) and Mn (manganese) concentrations were 37.02, 65.86, 14.79 and 44.93 mg^{-1} kg^{-1}, respectively, and mean grain protein was 13.76%. Application of the ANN models for predicting Zn, Fe, Cu, Mn and protein contents in grains improved prediction by 96.77%, 95.45%, 124.13%, 125% and 109.75%, respectively, over the multiple linear regression (MLR) models.The topographic parameters wetness index, plan curvature and shaded relief, selected soil properties total nitrogen (TN), soil organic matter, available phosphorus and DTPA-extractable micronutrients were identified as the most important parameters for explaining the variability in wheat grain quality at the study area.

Keywords: artificial neural network; grain micronutrients; protein; terrain parameters

Introduction

Micronutrients impact human health in several ways. Micronutrients such as iron (Fe), copper (Cu), manganese (Mn) and zinc (Zn) are essential micronutrients with a human requirement of no more than a few mg per day. Deficiency, excess or imbalances in the supply of minerals can harm human health (American Association of Cereal Chemist 1983; Ajoyi & Kamson 1983; Dwivedi et al. 2012).

Since wheat is the most important staple cereal in developing countries such as Iran, the concentration of micronutrients in grains plays a vital role in affecting human health. Wheat (*Triticum aestivum L.*) is the most important food crop and is grown under rain-fed conditions in many parts of the world, especially in the semiarid regions (Wahbi & Sinclair 2005; Yusefi et al. 2007; Norouzi et al. 2009).

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Several studies have been conducted to study micronutrient contents in grains depending on soil and climate conditions. Katyal and Sharma (1991) studied Zn, Cu, Mn and Fe concentrations in Indian soils and found that changes in pH, lime ($CaCO_3$), organic matter, size fractions (clay) and soil moisture regime had a strong influence on micronutrient distribution in the soil. Karami et al. (2009) performed a survey in central Iran to assess the variability in grain Zn, Fe and Cu concentration in winter wheat and their relationships with soil and climatic variables in the field. They showed that DTPA-extractable and total micronutrient concentrations in soil alone were poor predictors of grain micronutrient concentrations. The prediction was slightly improved when other soil and climate variables were taken into account.

The knowledge on the variability in grain micronutrient in staple cereals such as wheat in the semiarid regions of developing countries could provide valuable information for site-specific management within the landscape. Although some researchers (Karami et al. 2009) have used regression models to describe the relationships of soil and climatic properties with micronutrient contents, the use of artificial intelligence systems such as artificial neural networks (ANNs) has not been explored for this purpose. ANNs are computing systems made up of a number of simple, highly interconnected processing elements, also called neurons (e.g., Huading et al. 2007; Norouzi et al. 2009; Gago et al. 2010; Pradhan et al. 2011). Generally, an ANN is made of an input layer, one or several hidden layers (HLs) and an output layer of neurons. The input-layer neurons receive the information from the outside environment and transmit it to the hidden layer. Each neuron of a subsequent layer first computes a linear combination of the outputs from all neurons of the previous layer and then adds a bias to it. Furthermore, each neuron of an HL applies a specific nonlinear function, called activation function, to this linear combination plus bias. The coefficients of the linear combinations and the biases are called weights. Then, neurons in the HL apply a nonlinear function as activation function to their inputs (Bocco et al. 2010).

To the best of our knowledge, little attempt has been made to predict micronutrient concentration in wheat grain using topographic parameters as time and cost-efficient auxiliary variables. Topography plays a vital role in the field by shaping the spatial variability of soils, surface and subsurface hydrology, and crop yield (Iqbal et al. 2005). Therefore, the major objectives of this study were (1) to predict micronutrient (Zn, Cu, Mn and Fe) concentration in wheat grain using statistical approaches for geomorphometric analysis, (2) to compare the performance of ANN and MLR models and (3) to determine the most sensitive soil and topographic parameters that explain the variability in grain micronutrients as judged by sensitivity analysis, in the hilly regions of western Iran.

Materials and methods

Site description

The experimental site, 3600 ha in area, is located between 32° 20′ and 32° 30′ N latitude and 50° 14′ to 50° 24′ E longitude with approximately 2510 m a.s.l. in the Charmahal & Bakhtiari province, west of Iran (Figure 1). The long-term mean annual temperature is 9.4°C, and the average annual precipitation is 1400 mm, which falls mainly from November to May. Soil moisture and temperature regimes in this area are typic xeric and mesic, respectively, according to Soil Survey Staff (2006). The field sites are located on the hill-slopes about 20% transversal slopes with mainly Oligomiocene marl parent material. The soils at the site are classified as Vertisols, Entisols and Inceptisols according to soil taxonomy (Soil Survey Staff 2006) with dominant texture in the surface soil being clay.

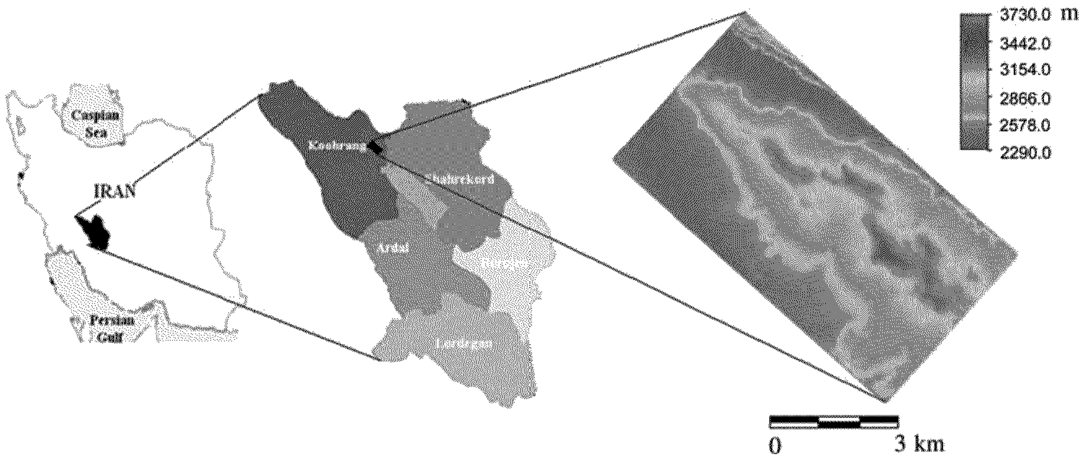

Figure 1. Location of the study area in Kohrang district, Charmahal & Bakhtiari, west Iran, along with the data of the digital elevation model (DEM). The scale bar is used for the DEM model.

Field survey and determination of soil and plant parameters

The fields selected have been cultivated for a long time with winter rain-fed wheat without any rotation, but with intermittent fallow years. Seedbeds at the site were prepared by chisel ploughing of each fall, followed by fertilizer application and sowing of the crop. Fertilizer was applied at the rate of 100-30-50 kg ha^{-1} N-P-K; and the date of planting of Sadri wheat cultivar was around 20 November 2010.

Slope positions were considered as the basis of sampling; 100 points distributed randomly stratified at all slope positions (summit, shoulder, backslope, footslope and toeslope) were selected for sampling. Twenty transects were selected about 1–3 km apart and within each transect sampling points were selected 100–300 m apart from each other. The crop was harvested around 15 July 2011 from the 100 selected plots (1 × 1 m^2); the harvested above-ground biomass was separated in grain and chaff after drying. Zinc, Fe, Cu and Mn concentrations in grain samples were determined using an atomic adsorption spectrometer (Perkin-Elmer model 430) after digestion of the ground samples with 5 N nitric acid (HNO_3) in the laboratory of Isfahan University of Technology (Ajoyi & Kamson 1983). N content in the grain samples was analyzed using the Kjeldahl method and wheat protein content was calculated using the following equation (American Association of Cereal Chemist 1983):

$$\% \text{ grain protein} = \% \text{ grain N} \times 6.25 \tag{1}$$

At harvest of the crop, surface (0–30 cm) soil samples were also collected from the same 100 points for laboratory analysis. Particle size distribution was measured using the hydrometer method (Gee & Bauder 1986). Calcium carbonate equivalent (CCE) was measured by the Bernard calcimetric method (Black et al. 1965). Soil organic matter (SOM) was determined using a wet combustion method (Nelson & Sommers 1982) and total N (TN) was determined by the Kjeldahl method. Available phosphorous (P_{ava}) was measured as described by Olsen and Sommers (1982). Extractable micronutrients in soils were determined using diethylene triamine pentaacetic acid (DTPA) as the extractant; Zn, Fe and Cu in the extract were determined using atomic absorption spectroscopy (Black et al. 1965). Soil pH was measured using a 1:2.5 soil/water ratio by a pH electrode (McLean 1982), and electrical conductivity (EC) was determined using an electrical conductivity meter (Rhoades 1982).

Topographic parameters

The topographic parameters, including slope, aspect, sediment transport index, shaded relief and wetness index,were determined using a 20 m by 20 m digital elevation model (DEM, see Figure 1). Moore and Hutchinson (1991) divided terrain parameters in two categories of primary and secondary (compound) parameters. Primary parameters are calculated directly using digital elevation models (DEMs) and included elevation (Elev), slope (Slop), aspect (ASP), catchment area (CA), plan curvature (PlanC), profile curvature (ProfC), tangential curvature (TangC) and shaded relief. Secondary or compound parameters involve combinations of the primary parameters and are used as indices that describe the spatial variability of specific processes occurring on the landscape such as soil water content or the potential for sheet erosion, wetness index (WI) and sediment transport index (STI). The definitions of selected topographic parameters are summarized in Table 1. The distribution of topographic parameters in the study area, derived from DEM, is illustrated in Figure 2. The descriptive statistics of terrain parameters for the 100 selected points are presented in Table 2.

Data analysis

Descriptive statistics of the experimental data including mean, minimum, maximum, range, coefficient of variation (CV), kurtosis and skewness were determined using the statistical software SPSS (IBM Com., Chicago, IL, USA). All the input data were normalized to a range of 0.1–0.9 using the following equation:

$$x_i = 0.8 \times \left[\frac{(x - x_{\min})}{(x_{\max} - x_{\min})}\right] + 0.1 \tag{2}$$

Each data set was then divided into three subsets of training, testing and verification. The training subset was randomly chosen from 60% of the total set of the data and the remaining samples (40% of the data) were used equally in two parts as the verification and validation sets.

Multiple linear regression (MLR)

Linear regression is one of the oldest statistical techniques, and has long been used in biological research (Guisan et al. 2002). The basic linear regression model has the following form:

$$Y = \alpha + X_T\beta + \varepsilon \tag{3}$$

where Y denotes the dependent variable, α is a constant called the intercept, $X = (X_1, \ldots, X_n)$ is a vector of explanatory variables, $\beta = \{\beta_1, \ldots, \beta_n\}$ is the vector of regression coefficients (one for each explanatory variable) and ε represents randomly measured errors as well as any other variation not explained by the linear model. In this study, the statistical software SAS (Cary, NC, USA) was used to determine the MLR models (Ayoubi et al. 2009). Soil and topographic parameters were selected as independent variables and grain micronutrient and protein contents were used as dependent variables in the models. These regression models were validated with the same dataset used in the validation of ANN models so that the results could be compared.

Table 1. Definition of topographic attributes (Moore et al. 1991; Florinsky et al. 2002).

Variable	Unit	Definition
Aspect (A)	degree	Direction of the maximum rate of change in the elevation from each cell of the digital elevation model (DEM), so that aspect is the direction of gradient. It influences the direction of substance flows.
Catchment area (CA)	m^2	Area draining to the catchment outlet
Elevation	m	Elevation above sea level.
Plan curvature (PLANC)	m^{-1}	Curvature of a surface perpendicular to the direction of the steepest slope. It is a measure of the convergence or divergence and thus indicates water content.
Profile curvature (PROFC)	m^{-1}	Curvature of a surface in the direction of the steepest slope. It is a measure of the rate of change of the potential gradient, and hence is important for water flow and sediment transport processes. It decelerates substance flow.
Sediment transport index (STI)	–	This accounts for the effects of topography on erosion and soil loss. $STI = \left(\frac{As}{22.13}\right)^{m}\left(\frac{\sin\beta}{0}.089\right)^{n}$, where As is specific area, β is slope degree, and m and n are constants.
Shaded relief	–	Simulates the cast shadow thrown upon a raised relief map, or more abstractly upon the planetary surface represented.
Slope (S)	%	Maximum rate of change in elevation from each DEM cell. It is the gradient at a specified point, and is used to identify the steepest of the gradients between a point and its neighbours. It shows the velocity of substance flows.
Specific catchment area (SCA)	$m^2\ m^{-1}$	Upslope area per unit width of contour, and it is the ratio of an area of an exclusive figure formed by a contour intercept with a given point on the land surface and is a measure of the contributing area.
Tangential curvature (TangC)	m^{-1}	Plan curvature multiplied by the slope.
Wetness index (WI)	–	Sets catchment area in relation to the slope gradient. It has been used to characterize the spatial distribution of zones of surface saturation and soil water content in landscapes. It shows the extent of flow accumulation. WI =ln $\left(\frac{As}{\tan\beta}\right)$, where As is the specific area and β is slope degree

Artificial neural networks (ANNs)

For neural network analysis, we used the multilayer perceptron (MLP) with the back-propagation (BP) learning rule, which is the most commonly used neural network structure in ecological modelling and soil science (Bocco et al. 2010; Pradhan et al. 2011). As the output of the MLP network, the micronutrient concentration (MC) was calculated as follows:

$$MC = f_2\left\{B_0 + \sum_{k=1}^{n}\left[w_k f_1\left(B_{Hk} + \sum_{i=1}^{m}[w_{ik}P_i]\right)\right]\right\} \tag{4}$$

where B_0 is the bias at the output layer; w_k is the weight of connection between neuron k of the hidden layer and the single output layer neuron; B_{Hk} is the bias at neuron k of the hidden layer (k = 1,…,n); w_{ik} is the weight of connection between the input variable i (i = 1,...,m) and neuron k of the hidden layer; P_i is the input variable i; $f_1(h_k)$ is the transfer function of the neurons in the hidden layer and $f_2(h_k)$ is the transfer function of the neuron

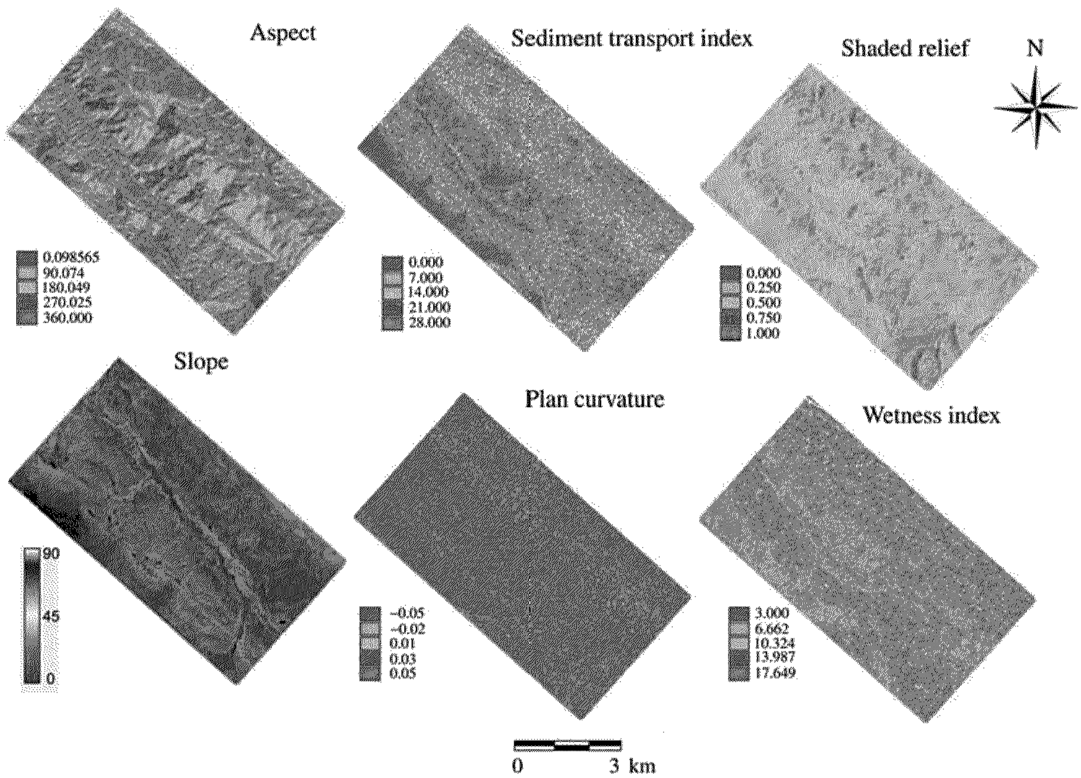

Figure 2. Spatial distribution of the topographic parameters at the site studied for predicting wheat grain micronutrients and protein.

Table 2. Summary statistics for the terrain attributes at the studied site (n = 100).

Variable	Unit	Minimum	Maximum	Mean	Skewness	Kurtosis	Range
Aspect	Degree	1.00	359.89	210.97	–0.43	–0.72	358.89
CA	m^2	100.06	69,539.54	2531.44	0.89	0.98	69,439.54
Elevation	m	2337.30	2773.40	2510.44	0.61	1.22	436.10
PLANC	m^{-1}	–0.04	0.05	–0.58	0.44	2.09	0.09
PROFC	m^{-1}	–1.28	1.01	0.013	–0.39	4.70	2.29
STI	–	4.84	44.90	24.87	0.87	2.90	40.06
Shaded relief	–	0.22	0.73	0.47	0.47	–1.27	0.51
Slope	%	0.00	21.17	10.58	0.62	0.85	21.17
SCA	$m^2\ m^{-1}$	99.21	852.00	365.00	–0.51	1.88	752.79
TangC	m^{-1}	–1.78	1.22	0.03	–0.68	3.01	3.00
WI	–	3.39	12.00	7.69	0.83	1.20	8.61

Notes: CA: catchment area; TangC: tangential curvature; PLANC: plan curvature; PROFC: profile curvature; STI: sediment transport index; WI: wetness index; SCA: specific catchment area.

in the output layer. Both transfer functions $f_1(h_k)$ and $f_2(h_k)$ adopted were sigmoid functions in this study, and can be represented by the following equation:

$$f_N(\lambda) = \frac{1}{1 + e^{-\lambda}} N = 1,2 \tag{5}$$

$$\lambda = P_i.w_i$$

where P_i is the input variable and the w_i is the weight of connections between layers. The numbers of neurons and epochs were determined by trial and error. Neural network analyses were performed using MatLab 7.6, Neural Networks Toolbox (Mathworks, Inc., Natick, MA, USA). To identify the most important soil and terrain parameters, sensitivity analysis was carried out using the Statsoft method (Statsoft Inc. 2004). A sensitivity ratio was calculated by dividing the total network error, when the variable was treated as being not variable, and by the total network error when the actual values of the variable were used. A coefficient greater than 1.0 implied that the variable contributed to a great extent to the variability of the target variable.

Evaluation criteria

The performance of the developed models can be compared using various standard statistical performance evaluation criteria. In the present study, the statistical measures considered include the root mean square error (RMSE) and the correlation coefficient between the measured and predicted micronutrients values, and they were used to evaluate the performance of the models using the following equation:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} [P(x_i) - M(x_i)]^2} \tag{6}$$

where $P(x_i)$ denotes the predicted value of observation i, $M(x_i)$ is the measured value of observation i and n is the total number of observations. The model had the lowest RMSE, and the highest coefficient of determination (R^2) was selected as the best-fit model.

Results and discussion

Descriptive statistics

The descriptive statistics of protein and micronutrient concentrations in grains, and soil parameters are given in Table 3. All variables were normally distributed according to the Kolmogorov–Smirnov (KS) test. The significant values of the KS test for all variables greater than 0.05 are presented in Table 3. Skewness values, which ranged from –1 to +1 (Table 3), also confirmed that all the variables were normally distributed. The mean values of Zn, Fe, Cu, Mn and protein in wheat grain were 30.70, 65.9, 14.8, 44.9 mg^{-1} kg^{-1} and 13.8%, respectively. It was observed that 61% of our samples had a Zn concentration higher than 24 mg^{-1} kg^{-1} dry matter, a critical value for Zn as suggested by researchers in Pakistan (National Research Council 1989) for alkaline soils for rain-fed wheat as the minimum grain Zn concentration required to produce 95% of the maximum grain yield. Based on our knowledge of the relevant literature, no critical values for other elements in wheat grains are available to compare our results with.

Skrbiic and Onjia (2007), in a study of 14 regions of Serbia, reported mean values of 33.2, 80.7, 5.30 and 50.90 mg^{-1} kg^{-1} for Zn, Fe, Cu and Mn in grains, respectively. In a study in central Iran from 137 samples in Fars, Isfahan and Qom provinces, Karami et al. (2009) found that grain micronutrient concentrations ranged from 11.7 to 64.0 mg kg^{-1} (mean 31.6 mg kg^{-1}) for Zn, from 21.1 to 96.6 mg kg^{-1} (mean 42.7 mg kg^{-1}) for Fe and from 2.4 to 9.3 mg kg^{-1} (mean 5.5 mg kg^{-1}) for Cu.

CV was calculated to describe the variability in selected variables. The CVs were 44%, 45%, 49%, 39% and 61% for Zn, Fe, Cu, Mn and grain protein, respectively (Table 3).

Table 3. Summary statistics of wheat grain Fe, Zn, Cu, Mn concentration and protein percentage and soil parameters (0–30 cm depth) for the site studied (n = 100).

Variable	Unit	Mean	Minimum	Maximum	Skewness	Kurtosis	Range	CV (%)	KS value
Grain data									
grain Cu	mg kg^{-1}	14.8	10.2	21.3	0.19	0.34	11.0	49	0.2
grain Fe	mg kg^{-1}	65.9	49.6	90.1	0.3	1.2	40.5	44	0.2
grain Mn	mg kg^{-1}	44.9	35.6	72.4	0.9	2.1	36.8	39	0.2
grain protein	%	13.8	8.7	18.8	–0.4	–1.6	10.0	61	0.2
grain Zn	mg kg^{-1}	30.7	12.7	48.7	0.3	1.3	36.0	45	0.2
Soil properties									
DTPA-Cu	mg kg^{-1}	1.5	0.2	2.7	0.6	0.4	2.5	65	0.2
DTPA-Fe	$mgkg^{-1}$	11.8	1.4	22.3	0.2	1.2	20.9	63	0.2
DTPA-Mn	mg kg^{-1}	25.3	4.1	46.6	0.3	0.1	42.4	46	0.1
DTPA-Zn	mg kg^{-1}	1.7	0.8	2.6	0.9	0.2	1.7	70	0.1
CCE	g kg^{-1}	386	120	652	0.7	1.8	532	98	0.2
Clay	g kg^{-1}	435.0	320.0	550.0	–0.2	1.2	230.0	32	0.1
EC	dS m^{-1}	1	0.3	1.7	–0.1	–2.3	1.3	30	0.2
P_{ava}	mg kg^{-1}	31.3	2.5	60.2	0.8	1.5	57.6	43	0.2
pH	–	7.6	7.3	8.0	0.6	1.9	0.6	1.3	0.2
Sand	g kg^{-1}	280.0	45.0	515.0	0.9	3.4	470.0	35	0.2
SOM	g kg^{-1}	10.9	2.0	19.8	0.5	0.3	17.7	45	0.2
TN	g kg^{-1}	3.3	0.3	6.3	0.6	2.1	5.9	88	0.2

Notes: TN: total nitrogen; SOM: soil organic matter; P_{ava}: available phosphorous; EC: electrical conductivity. CV: coefficient of variation; KS value: Kolmogorov–Smirnov value test.

The CV values of yield components might have been affected by diverse fertilization practices within the hill-slope, management practices and the diversity of field topography (Kravchenko et al. 2005). Whelan and McBratney (2000) observed that the CV of wheat yield and nutrient contents varied from 13% to 83% within the field.

Soil properties showed relatively higher variation than grain protein and micronutrient concentrations. Their CV value ranged from 1.3% for pH to 98% for CCE. The variability in soil properties depends on the topography of the field and the landscape position, causing differential accumulation of water, and consequently nutrients, at different positions in the landscape.

Multiple linear regression (MLR) analysis

Stepwise linear regression was performed among grain micronutrient and protein contents and soil and topographic parameters. The topographical and soil parameters used in the multiple regression equations included soil extractable micronutrients, TN, SOM, CCE, WI and slope (Table 4). In the final stepwise multiple regression equations, WI appeared with a positive effect, and this parameter was mainly responsible for regression. Slope had a negative effect on all selected target variables because of erosional effects on soil nutrients, and negative impact of slope position on water availability. Moreover, CCE

Table 4. MLR models developed for predicting wheat grain micronutrients and protein using soil and topographic attributes.

Target variable	Developed equation	R^2	P value
grain protein	0.011 + 0.23 TN + 0.09 SOM + 0.11 WI	0.41	0.002
grain Zn	0.009 + 0.12 DTPA-Zn + 0.08 SOM + 0.2 WI-0.05 Slope	0.31	0.02
grain Cu	0.013 + 0.112 DTPA-Cu + 0.02 SOM + 0.11 WI-0.04 Slope	0.29	0.03
grain Fe	0.11 + 0.04 DTPA-Fe + 0.07 SOM-0.13 CCE + 0.145 WI	0.22	0.04
grain Mn	0.08 + 0.12 DTPA-Mn + 0.11 SOM + 0.21 WI-0.06 Slope	0.36	0.015

Notes: TN: total nitrogen; CCE: calcium carbonate equivalent; SOM: soil organic matter; WI: wetness index.

was identified as the factor that reduced Fe content in wheat grains (Table 4). MLR models for predicting grain Zn, Fe, Cu, Mn and protein contents by soil and topographic parameters resulted in values of coefficient of determination (R^2) of 0.31, 0.22, 0.29, 0.36 and 0.41, respectively (Table 4). Karami et al. (2009) showed that the inclusion of soil and climatic variables using MLR models in central Iran could explain only 29%, 8% and 13% of the total variability in grain Zn, Fe and Cu contents, respectively. The MLR models for protein, Zn, Fe, Cu and Mn contents in wheat grain at the studied site resulted in RMSE values of 0.05, 0.03, 0.02, 0.03 and 0.10, respectively. Yang et al. (1998) reported that three topographic parameters – elevation, slope and aspect – could explain 15–35% of wheat yield variability at the field scale.

These results indicated that in arid and semiarid regions, the primary effect of topographical factors on grain nutrients and protein was probably related to water availability during the growth season. WI indicates the distribution of drier and wetter zones in the landscape (Moore, Gallant, et al. 1993). From our results, 49–78% of the variability in grain micronutrient and protein contents remains unexplained. For further evaluation of the variability, we used ANN models for predicting selected variables in this study.

Artificial neural networks (ANNs) analysis

Table 5 shows the best structure and optimum parameters of the final selected ANN models that were used to predict wheat grain micronutrients and protein concentrations. Each of the trained structures had 22 input nodes – including soil and topographic parameters – and one output node. The hidden-layer nodes optimized were 25, 22, 23, 22 and 25 and the optimum iteration learning rates based on trial and error at 9000, 6000, 10,000, 8000, 8000 and 7000 for Zn, Fe, Cu, Mn and protein contents in grain, respectively. ANN models resulted in R^2 and RMSE of 0.61 and 0.02 for Zn concentration, 0.43 and 0.003 for Fe concentration, 0.65 and 0.001 for Cu concentration, 0.81 and 0.001 for Mn concentration, and 0.86 and 0.001 for protein content of wheat grain in the study area.

Unaccounted variability in the case of the ANN model indicated that other factors – such as environmental factors, fertilization and management practices along with the landscape – play significant roles in plant metabolism, uptake of micronutrients and synthesis of grain protein (Dick et al. 1985). Other reasons for the unexplained variability might be attributed to inadequate understanding of micronutrient transfer within the plant, from root to shoot and consequently to grain.

Table 5. Summary of the results on structure and optimum parameters for the best fit of the artificial neural network (ANN) model.

Components	Transfer function	Epochs	Number of input parameters	Number of hidden neurons	RMSE	R^2
grain Zn	Tansigm	9000	22	25	0.02	0.61
grain Fe	Tansigm	6000	22	22	0.003	0.43
grain Cu	Tansigm	10,000	22	23	0.001	0.65
grain Mn	Tansigm	8000	22	22	0.001	0.81
grain Protein	Tansigm	7000	22	25	0.001	0.86

Notes: R^2: coefficient of determination; RMSE: root mean square error. Tansigm: tangential sigmoid transfer function; Epoch: the numbers used by training protocol to spin before convergence is achieved.

Comparison of the MLR and ANN techniques

Based on the values of R^2 and RMSE (Tables 4 and 5), it appears that MLR models had lower efficacy to predict grain Zn, Cu, Fe, Mn and protein concentrations than the ANN models. In general, using the ANN models the predicted micronutrient and protein concentrations were found to be in better agreement with the observed values than those predicted using the MLR models. Linear multiple regression models were unable to predict a large proportion of total variability in grain micronutrient concentrations, presumably because the effects of the predictors on the dependent variables might not be linear in nature. A reason for these findings could be attributed to the nonlinear relationships among the soil and topographic parameters, and the grain micronutrient concentration; moreover, the ANN technique can estimate such relationships using nonlinear functions. The lower accuracy of the MLR approach might also be due to sample distribution, spatial variation and the scale effects at the study area.

Application of ANN modelling improved the coefficients of determination for the concentrations of Zn, Fe, Cu, Mn and protein content in grains by 96.77%, 95.45%, 124.13%, 125% and 109.75%, respectively. Our results are in agreement with those reported by others. Kaul et al. (2005), for instance, compared the MLR and ANN models for predicting corn and soybean yields and reported that the ANN models consistently gave more precise yield predictions than the regression models. Huading et al. (2007) found that a combination of geographical information system (GIS) and neural networks was useful for assessing wind erosion hazard in Inner Mongolia, China. Bocco et al. (2010) evaluated the potential use of linear models and neural networks in estimating solar radiation, and reported better results using neural networks. Gago et al. (2010) concluded that ANNs are a useful alternative to the traditional statistical methodology for analyzing plant data.

ANN application has functional characteristics and provides several advantages over the MLR approach. The most important advantage of using the neural network approach is that the network is trained to find the nonlinear relationships among variables. Moreover, powerful parameters of ANN models are flexible and adaptable, which play an important role in material modelling.

Sensitivity analysis

After the final selection of ANN models, sensitivity analysis was performed to evaluate the relative importance of each variable in explaining grain components. The results of sensitivity analysis and distribution of sensitivity coefficients for the selected variables are presented in Figure 3.

Among the topographic parameters, WI, plan curvature and shaded relief were identified as the most important factors for grain micronutrient concentration and protein content (Figure 3). WI and plan curvature had a great impact on the quality of wheat grain in the study area. Plan curvature, which is the curvature in the horizontal plane of the contour line, measures topographic convergence and divergence, and hence the propensity of water to converge as it flows across the land (Wilson & Gallant 2000). Therefore, this parameter, to a great extent, determines the kind of flow across the land, the soil properties and the amount of soil water content, especially in arid and semiarid regions. Sinai et al. (1981) showed that in arid regions, soil water content was highly correlated with soil surface curvature. In semiarid regions under rain-fed conditions, soil water is the major limiting factor for crop production; moreover, the processes that control soil water distribution also control crop production (Si & Farrell 2004). Water accumulation and runoff processes are largely determined by landscape configuration (Si & Farrell 2004).

Shaded relief has been used to estimate solar radiation (Moore, Gallant, et al. 1993) and hence spatial distribution of soil physical and chemical properties (Moore, Lewis, et al. 1993). Shaded relief is also one of the other most important topographic parameters

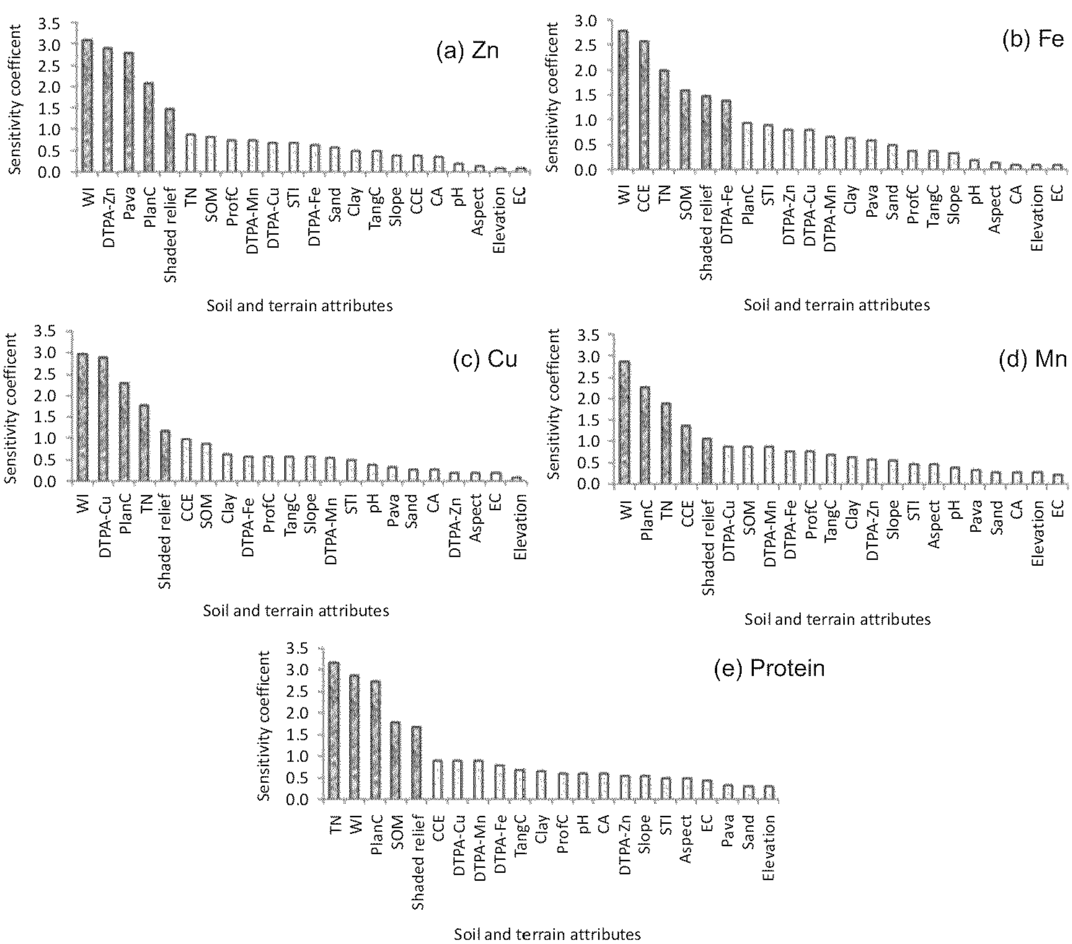

Figure 3. Relative sensitivity coefficients of soil and topographic parameters for wheat grain (a) Zn, (b) Fe, (c) Cu, (d) Mn and (e) grain protein for the study area in western Iran. For details of abbreviations, see Tables 1 and 3.

that control soil temperature (Wilson & Gallant 2000) and thus could indirectly influence crop yield and quality. Dick et al. (1985), Kabata-Pendias and Pendias (2001) and Karami et al. (2009) reported that soil temperature greatly affects nutrient uptake.

Among the soil properties, TN, CCE, P_{ava}, SOM and DTPA-extractable micronutrients were identified as the most important soil factors explaining the variability in grain micronutrients. Other studies (Rashid & Ryan 2004; Alvarez et al. 2006; Obrador et al. 2007; Schulin et al. 2008) showed that soil properties such as micronutrient concentration, CCE, organic matter, soil moisture conditions and available P control the phytoavailability of soil micronutrients by plants. There is some indication that additional P in soil reduces the solubility and phytoavailability of Zn, thus potentially limiting uptake by root and affecting grain Zn (Alloway 2004, 2008; Lambert et al. 2007; François et al. 2009).

Several researchers (Morgounov et al. 2007; Shi et al. 2010) reported that the management of N fertilizer could affect the micronutrient concentration in grains. For example, Morgounov et al. (2007) found a strong correlation between Fe and Zn, and protein content. The results presented in Figure 3 indicate that the phytoavailability of micronutrients in soils could significantly affect grain micronutrients. These findings are also consistent with the findings of Krauss et al. (2002) and Nan et al. (2002). Krauss et al. (2002) reported a close relationship between EDTA-Zn and wheat grain Zn and a weaker relationship between EDTA-Cu and grain Cu.

Although various studies (Dick et al. 1985) showed that soil pH had a significant effect on micronutrient availability, especially Fe and Mn in cereal grains, in our study soil pH did not explain considerable variability of nutrients in wheat grain.This is presumably ascribed to the low variability of soil pH (CV = 1.3%) in the study area, which probably did not influence the variability of micronutrients in soils and consequently in plant and grain.

Overall, the results indicated that ANN models were better in predicting wheat grain quality using soil and topographic parameters. These results are consistent with the findings of Ayoubi and Sahrawat (2011); these authors also compared the MLR and ANN techniques to predict barley production using soil characteristics in northern Iran.

Conclusion

It is concluded that the land topography controls the contents of micronutrients and protein in wheat grain through its effects on soil properties such as soil moisture, temperature, soil organic matter, calcium carbonate content and clay, which in turn control plant growth and availability of nutrients in the soil. The results further revealed that easily accessible, quantitative topographic data such as digital elevation models (DEMs) could be used to predict grain quality at the hill slope scale, especially by employing nonlinear ANN modelling in combination with soil properties. It is suggested that the inclusion of management information along with these parameters might further improve the prediction using the ANN models.

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