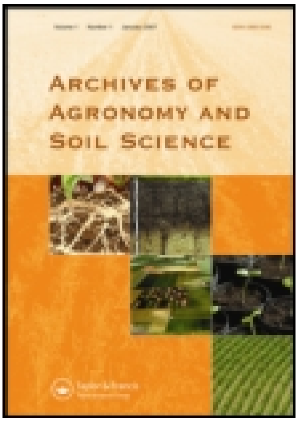

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Estimation of bulk density of waterlogged soils from basic properties

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Estimation of bulk density of waterlogged soils from basic properties

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Pedotransfer functions (PTFs) to predict bulk density (BD) from basic soil data are presented. Available data pertaining to seasonally impounded shrink–swell soils of Jabalpur district in the Madhya Pradesh state of India were used for the study. The data included horizon-wise information of 41 soil profiles in the study area covering nearly 5 million ha. Six independent variables, namely textural data (sand, silt and clay), field capacity (FC), permanent wilting point (PWP) and organic carbon content (OC) were used as input in hierarchical steps to establish dependencies, with bulk density as the dependent variable, using statistical regression and artificial neural networks. The PTFs derived using neural networks [average root mean square error (RMSE) 0.05] were relatively better than statistical regression PTFs (average RMSE $>$ 0.1). The best-performing PTFs required input data on sand, silt content, FC and PWP, with lowest prediction errors (RMSE 0.01, maximum absolute error (MAE) 0.01) and highest values of index of agreement (d, 0.95) and R^2 (0.65). Use of measures of structure, as well as information on pore structure, was found to be essential to derive acceptable PTFs. Inclusion of OC as an input variable showed relatively better fitting to the training data set, implying an underlying relationship between OC and BD, but the neural networks could not mimic the relationship when tested against subset.

Keywords: bulk density; neural networks; pedotransfer function; waterlogged soils

Introduction

An assessment of the dynamic behaviour of soil forms an integral base of land use plans. Therefore, simulation models of soil dynamics are increasingly gaining credence in complex assessments. Many of the models concerned with water and solute movement in the vadose (unsaturated) zone require soil bulk density (BD) and particle density as basic input parameters to further calculate water retention and hydraulic conductivity parameters (Leonavièiûtë 2000). Information on soil BD is indispensable for the assessment of soil carbon stocks and nutrient pools (Tamminen and Starr 1994). It is considered to be a key property that characterizes soil structure in general. BD has been found to correlate negatively with root density and tree growth (Salifu et al. 1999). However, data on soil physical properties are often inadequate in India, primarily due to the high expenses, time and manpower required for intensive or systematic sampling to obtain spatially distributed soil data. There is a need to derive algorithms to predict basic soil physical parameters like BD from easily available or

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easily measured data such as particle size distribution and/or organic matter/ carbon.

Indirect methods to derive required soil parameters from easily measurable input data are called pedotransfer functions (PTF; Bouma and Van Lanen 1987). Different types of BD PTFs have been calibrated using different approaches (Rawls 1983; Hollis et al. 1995). Soil physical and chemical data have been used as inputs in most of the studies (Saini 1966; Rawls 1983; Manrique and Jones 1991; Baumer 1992; Bernoux et al. 1998; Calhourn et al. 2001). These studies focused on a specific or limited data set. Most of the published PTFs use soil textural composition and/or organic carbon/matter data as input variables in an attempt to utilize limited available soil survey information (Curtis and Post 1964; Rawls 1983; Huntington et al. 1989; Benites et al. 2007). Bulk density has been found to vary with depth (Harrison and Bocock 1981; Huntington et al. 1989; Leonavièiûtë 2000), soil group (Alexander, 1980; Manrique and Jones 1991; Salifu et al. 1999), land use and vegetation (Harrison and Bocock 1981). Studies also indicate that BD can be better predicted with limited input data. For example, Benites et al. (2007) calibrated PTFs to predict BD in Brazilian soils using 17 different properties and concluded that the PTFs based on clay content, total nitrogen and sum of basic cations were superior to others using extended inputs.

PTFs have limited use outside the area of development due to their empirical nature. There are no PTFs that could be termed global (Tietje and Tapkenhinrichs 1993). Recent publications also corroborate that the applicability of BD PTFs outside the area of development must be examined carefully. For example, De Vos et al. (2005) evaluated the predictive quality of 12 published PTFs to estimate BD of forest soils in Belgium. The evaluation demonstrated poor performance of some published PTFs, and raised concerns that the predictive ability of even the better models may not be adequate. They also recalibrated and validated PTFs using native data. Harrison and Bocock (1981) recommended that to obtain a high degree of accuracy and great precision in estimating soil BD, an equation specific for each range of soils of relevance to a particular research program should be used, rather than relying on general PTFs. However, PTFs calibrated using native data may not represent the dependencies accurately, as reported by Kätterer et al. (2006). The best PTFs calibrated by them could only explain 40–43% of the total variance with corresponding root mean square error (RMSE) values of 0.14 g cm^{-3} and 5.3% by volume, respectively.

To overcome the constraints of PTF validity, Schaap and Leij (1998) suggested choosing those PTFs that correspond to the soil data sets of a similar geographical and geological region. They also opined that those selected PTFs still must be calibrated, tested and evaluated on the measurements of local soils to make sure that PTFs predictions are applicable.

Following on from these studies, we hypothesized that PTFs calibrated using native data would be more precise than the published PTFs. The objectives of our study were to: (1) calibrate PTFs to estimate BD, and (2) evaluate proposed PTFs against subset. We would like to add here that, to the best of our knowledge, no calibration or evaluation of PTFs for estimating the BD of seasonally impounded soils have been reported from India. The agricultural productivity of these soils is limited to only one winter crop subject to timely drainage after recession of monsoons and the quantum of residual moisture. For better management of these soils, it is necessary to understand their characteristics.

Materials and methods

Seasonally impounded shrink–swell soils occupy nearly 5 million ha (50% of geographical area) of Jabalpur district in central India (Rajput et al. 2004). From an agricultural perspective, these soils are difficult to manage. The area receives on an average of 1300–1500 mm rainfall, mostly during the rainy season. Because the soils remain waterlogged in the monsoon season, an agricultural crop is possible only in the rabi season after recession of the monsoon (October–December). The soils of the area are clayey and classified as Vertisols and Vertic intergrades (Inceptisols). The dominant series of this area are Sihora and Kunda, characterized as fine, smectitic, hyperthermic Typic Haplusterts and fine, smectitic, hyperthermic Vertic Haplustepts (Tomar et al. 1996). Being poorly drained soils and encouraged by topography, the water stagnates in the fields during monsoon. Farmers have devised a 'Haveli' system, which brings the farming community together to build bunds in each field to impound water during the monsoon. The water is released systematically 15 days after the recession of rainfall and residual moisture is utilized to grow different crops. This practice is believed to be more than 150 years old. Years of impounding has imparted special characteristics to the soils. Data on basic properties were collected by sampling 41 profiles. The 'Haveli' tract was traversed to mark representative sites (depending on soil variability) and the profiles were cut open to collect stratified bulk samples from 174 horizons. Clay, clay loam and sandy clay loam texture were recognized in 102, 18 and 22 horizons, respectively (USDA classification). These three textures constituted 82% of the entire data set. The remainder of the 32 horizons was dispersed over textures; loam (10), silty clay (10), silty clay loam (4), sandy loam (3), sandy clay (3) and silt loam (2). Investigations reported here are limited to the clay horizons because no adequate data for other textures was available for developing PTFs. For more details the reader is referred to Patil and Rajput (2009). A statistical summary of the physical properties data is shown in Table 1. The soils were predominantly clayey (40.5–71.5%) in texture. The mean sand and silt content of the soils were almost identical, but sand fraction varied greatly [coefficient of variation (CV) 0.4] in comparison with the other two fractions. Bulk density did not vary much with a mean value of 1.4 g cm^{-3}.

The soil properties selected for this study were: full soil particle size distribution, field capacity (FC), permanent wilting point (PWP) and soil bulk density (BD). These soil properties were chosen because the data on them is usually available in many soil reports, and because other authors have reported utility in their works for deriving PTFs.

Table 1. Statistical summary of basic properties of 102 clay soil samples.

	Sand (%)	Silt (%)	Clay (%)	FC (%)	PWP (%)	BD (g cm^{-3})
Mean	20.5	25.5	53.5	0.3	0.2	1.4
SE	0.9	0.5	0.9	0.0	0.0	0.0
SD	8.8	5.5	8.7	0.0	0.0	0.1
CV	0.4	0.2	0.2	0.1	0.2	0.1
Minimum	3.1	8.0	40.5	0.2	0.1	1.2
Maximum	36.7	39.1	71.5	0.4	0.2	1.7

Notes: BD, bulk density; CV, coefficient of variation; FC, field capacity; PWP, permanent wilting point; SD, standard deviation; SE, standard error.

Deriving PTFs

Statistical and neural regression PTFs were derived. Eleven levels of input information were identified to establish dependencies between basic soil properties and BD. Logarithmic transformation was applied to the BD values for better representation of the data.

Input level 1	Textural data (data on sand, silt, and clay fraction – SSC)
Input level 2	Level 1 + organic carbon (1 + OC)
Input level 3	Level 2 + field capacity (2 + FC)
Input level 4	Level 3 + permanent wilting point (3 + PWP)
Input level 5	Data on sand, silt, OC, FC and PWP
Input level 6	Data on sand, silt, OC and FC
Input level 7	Data on sand, silt and OC
Input level 8	Data on sand, silt, clay and FC
Input level 9	Data on sand, silt, clay, FC and PWP
Input level 10	Data on sand, silt and FC
Input level 11	Data on sand, silt, FC and PWP

Based on earlier experience (Patil et al. 2010), a feed-forward neural network (FF-NN) model with three hidden nodes was preferred. According to Maier and Dandy (2000), feed-forward neural networks (FF-NN) are the most widely adopted network architecture for the prediction and forecasting of geophysical variables. Typical FF-NN consists of three layers – an input layer, a hidden layer and an output layer. The number of nodes in an input layer corresponds to the number of inputs considered for the PTFs. The input layer is connected to the hidden layer with weights that determine the strength of the connections. The hidden layer provides the network's non-linear modelling capabilities. As a general rule, the hidden units should be half the number of input units. Thus, in the present analysis, the maximum number of inputs being seven, three hidden units were considered optimum. The data sets were partitioned into 'training' (76 samples) and 'test' (26 samples) sets. Upon finding an appropriate network model, the PTFs were derived. For network training, the Levenberg–Marquardt (L–M) algorithm was chosen because the data set was small. Mayr and Jarvis (1999), Van Genuchten and Leij (1992) and other researchers used the same algorithm to develop PTFs. Further, for fair comparison between statistical regression and artificial neural network based PTFs (ANN–PTFs), it was desirable to seek minimization of sum of squares error.

Performance evaluation

Performance of the PTFs was evaluated based on one-to-one correspondence between measured and predicted values of BD. Statistical indices used for the evaluation were root mean square error (RMSE), regression coefficient (R^2), mean absolute error (MAE), degree of agreement (d) and maximum error (ME). These are based on squared difference between measured (M_i) and estimated (E_i) value, where 'i' indicates the ith value of a data set containing 'n' values. The degree/index of agreement is both a relative and bounded measure ($0 < d < 1$).

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(E_i - M_i)^2}{n}}$$

$$\text{Index of agreement } d = 1 - \frac{\sum_{i=1}^{n} (E_i - M_i)^2}{\sum_{i=1}^{n} \left(\left|E_i - \overline{M}\right| + \left|M_i - \overline{M}\right|\right)^2}$$

$$\text{Maximum absolute error ME} = Max|E_i - M_i|$$

Table 2. Regression PTFs to estimate bulk density and their performance as indicated by coefficient of determination (R^2).

PTF	R^2 (Fitting)	R^2 (Testing)
Log (BD) = 0.09045 + 0.0000172*Sand − 0.00071*Silt + 0.001584*Clay	0.18	0.13
Log (BD) = −1.2628 + 0.01409*Sand + 0.0134*Silt + 0.01516*Clay − 0.0675*OC	0.23	0.12
Log (BD) = −1.2595 + 0.0141*Sand + 0.0135*Silt + 0.0153*Clay − 0.0006*FC − 0.0663*OC	0.24	0.14
Log (BD) = −0.6862 + 0.0084*Sand + 0.0077*Silt + 0.0090*Clay − 0.0027FC + 0.0060*PWP − 0.0735*OC	0.40	0.12
Log (BD) = 0.2046–0.00049*Sand − 0.0001*Silt − 0.0717*OC − 0.0028*FC + 0.0066*PWP	0.36	0.06
Log (BD) = 0.2569–0.0010*Sand − 0.0016*Silt − 0.0602*OC − 0.0004*FC	0.17	0.21
Log (BD) = 0.2417–0.0009*Sand − 0.0016*Silt − 0.0612*OC	0.17	0.25
Log (BD) = 0.09649–0.0000317*Sand − 0.00071*Silt + 0.001568*Clay − 0.000013*FC	0.18	0.13
Log (BD) = 0.4515–0.00358*Sand − 0.00434*Silt − 0.00249*Clay − 0.00235*FC + 0.005976*PWP	0.30	0.32
Log (BD) = 0.251831–0.00158*Sand − 0.00226*Silt − 0.000014*FC	0.18	0.12
Log (BD) = 0.206618–0.00114*Sand − 0.0019*Silt − 0.00225*FC + 0.005755*PWP	0.30	0.32

Notes: BD, bulk density; FC, field capacity; OC, organic carbon; PWP, permanent wilting point.

Table 3. Statistical indices to judge performance of PTFs.

	Training					Testing				
PTF Input	RMSE	*d*	ME	MAE	R^2	RMSE	*d*	ME	MAE	R^2
SSC	0.02	0.81	0.05	0.02	0.52	0.03	0.59	0.08	0.03	0.13
SSC + OC	0.04	0.46	0.07	0.03	0.27	0.03	0.59	0.08	0.03	0.05
SSC + OC + FC	0.04	0.39	0.07	0.03	0.22	0.03	0.49	0.09	0.03	0.01
SSC + OC + FC + PWP	0.02	0.88	0.05	0.02	0.59	0.02	0.75	0.06	0.03	0.42
SS + OC + FC + PWP	0.04	0.67	0.06	0.03	0.64	0.02	0.86	0.05	0.02	0.35
SS + OC + FC	0.03	0.59	0.06	0.03	0.23	0.03	0.60	0.08	0.03	0.18
SS + OC	0.03	0.49	0.06	0.03	0.23	0.03	0.59	0.08	0.03	0.07
SSC + FC	0.04	0.18	0.09	0.03	0.01	0.05	0.19	0.09	0.04	0.05
SSC + FC + PWP	0.02	0.93	0.03	0.02	0.79	0.05	0.53	0.09	0.05	0.05
SS + FC	0.29	0.70	0.06	0.02	0.38	0.03	0.70	0.08	0.02	0.28
SS + FC + PWP	0.01	0.95	0.04	0.01	0.83	0.01	0.95	0.07	0.01	0.65

Notes: FC, field capacity; OC, organic carbon; PWP, permanent wilting point; SSC, sand, silt, clay content.

$$\mathrm{MAE} = \sum_{i=1}^{n} \frac{|E_i - M_i|}{n}.$$

Results and discussion

Statistical PTFs derived from the measured data are presented in Table 2. Evaluation of the performance of PTFs (Table 3 showed that the equations did not fit accurately to the data. This was evident from the testing data as well, which showed that correspondence between measured and estimated BD values was poor. Regression coefficient values in fitting to the measured data and testing with subset ranged from 0.12 to 0.32, indicating a poor performance of PTFs. Thus our attempt to utilize limited soil information did not succeed.

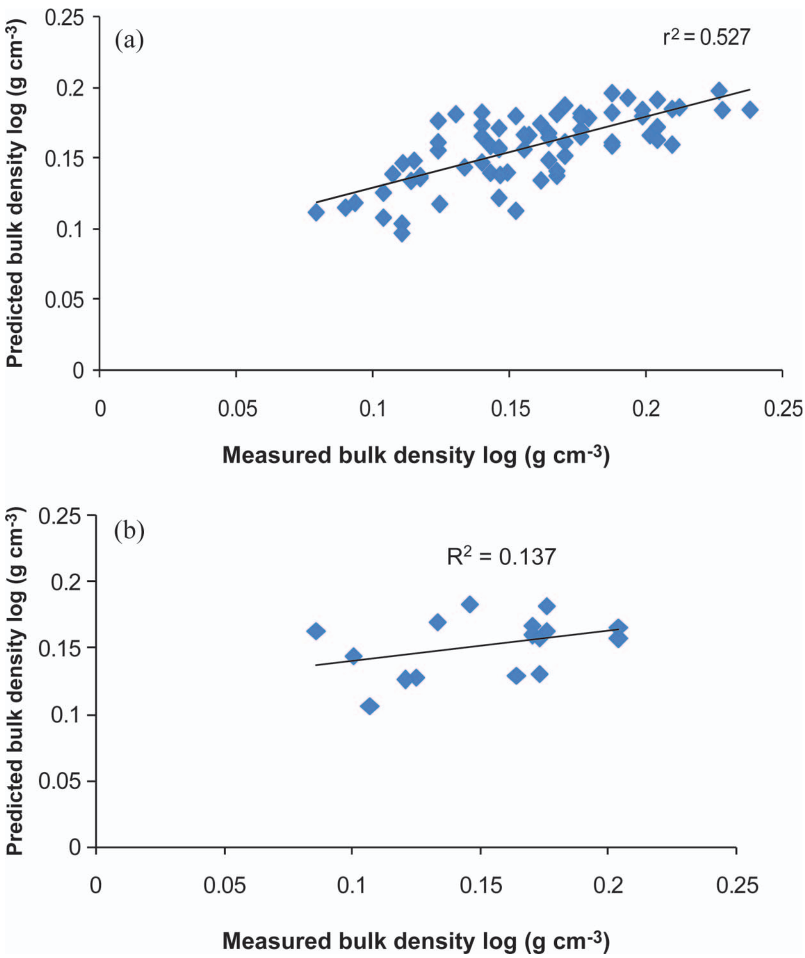

Figure 1. Correspondence between measured and predicted bulk density values with textural data as an input in a derived pedotransfer function (PTF): (a) training and (b) testing data set.

However, neural PTFs performed better than statistical PTFs. PTFs utilizing minimum information (sand, silt and clay) were of the lowest value, as indicated by the statistical indices (Table 3) for testing. It was observed that the networks fitted to the observed/training data well (Figure 1a with lower RMSE (0.02) and other errors, *d* (0.81) and R^2 (0.52). But, when tested against subset, the magnitude of error(s) increased (Figure 1b) with poor R^2 (0.05) and *d* (0.19). The neural networks are expected to improve in modelling ability with increase in number of input variables that are believed to affect the predicted property. However, with inclusion of FC as an input variable, the PTF performance declined. In fact, among all PTFs, this PTF using textural information and FC was observed to be of the lowest utility value. The highest prediction error was indicated by RMSE, R^2, ME and MAE values. FC is expected to provide better information on soil pore structure. However, the shrink–swell nature of the study soils was perhaps responsible for the inadequacy of neural networks in mimicking the effect on BD. Replacing FC by OC produced similar results, implying that texture and OC did not combine well to influence BD. These

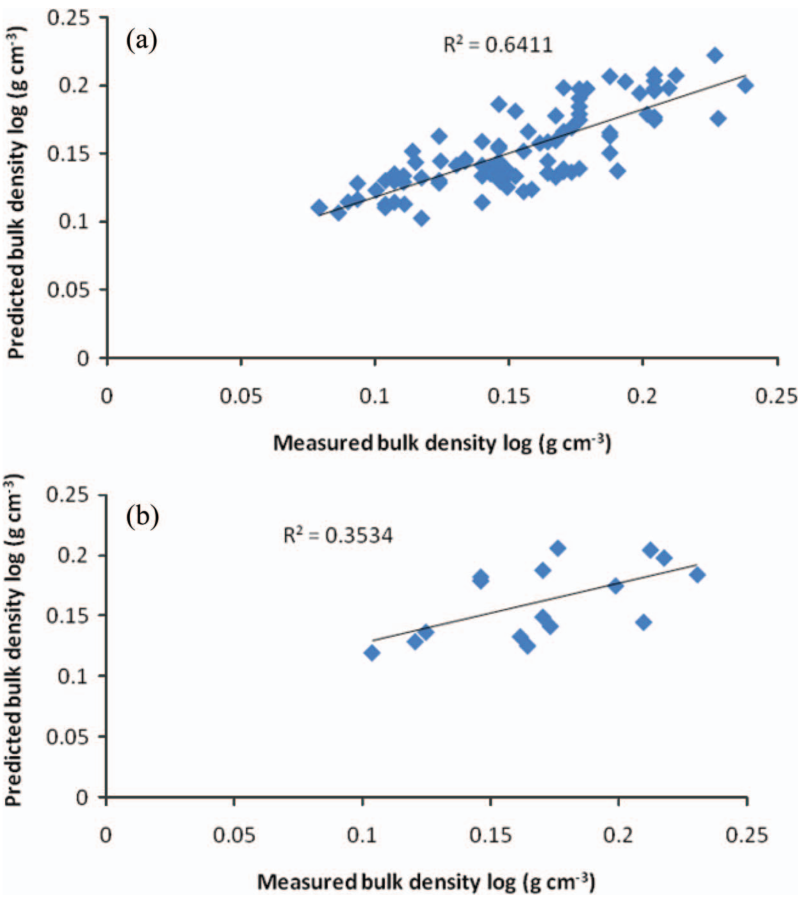

Figure 2. Correspondence between measured and predicted bulk density values with textural data, field capacity (FC), permanent wilting point (PWP) and organic carbon (OC) as an input in a derived pedotransfer function (PTF): (a) training and (b) testing data set.

soils are very poor in organic matter/carbon content, varying within a narrow range of 0.2–0.4%. It can be seen from Table 3 that the best performing PTFs were: (1) SS (sand, silt) + FC + PWP, and (2) SSC (sand, silt, clay) + OC + FC + PWP. OC content as an input showed some influence in combination with FC and PWP (Figure 2) or sand, silt and PWP (Figure 3) but it was not adequately expressed, perhaps owing to the narrow band of variation. The PTFs trained well but committed large errors in prediction. Against expectations, incremental addition of input variables in different combinations did not necessarily improve PTFs. The inability of the neural networks in predicting BD may also be due to an insufficient spread of the data or inadequate data for networks to mimic the underlying relationship.

Use of maximum number of variables (6) in PTF SSC + OC + FC + PWP recorded the second best RMSE (0.02) and a lower magnitude of other errors. The testing of PTF also showed better predictive ability. The best PTF required information on four variables namely sand, silt, FC and PWP. The networks trained

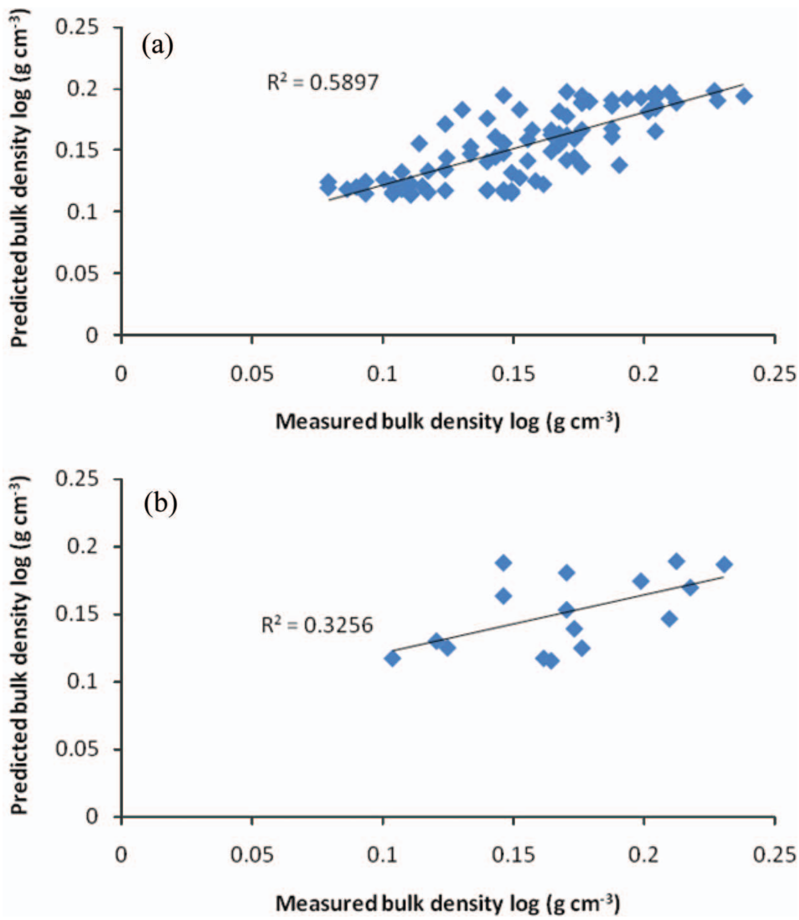

Figure 3. Correspondence between measured and predicted bulk density values with sand, silt, organic carbon (OC) and permanent wilting point (PWP) as an input in derived PTF: (a) training and (b) testing data set.

well when these data were used as input variables (Figure 4a) implying that the choice of input properties also influenced performance of neural regression. There was definite improvement in PTFs performance when FC and PWP were included in place of the clay fraction as an input. It could be argued that measures of structure, as well as information on pore structure, were essential to predict BD accurately. Exclusion of clay as an input variable led to improvement in PTFs performance probably because the clay content was always >40% with low coefficient of variation that caused difficulty in training networks. The best-performing PTFs (input sand, silt, FC and PWP) had the lowest RMSE (0.01), MAE (0.01), and the highest d (0.95) and R^2 (0.83) when networks were fitted to the measured data. It also had the lowest RMSE (0.01) and MAE (0.01), and the highest d (0.7) and R^2 (0.65) when tested for predictive ability.

Thus it was evident that PTFs to predict BD of the impounded shrink–swell soils could be used to obtain reasonable estimates with a relatively higher number of input variables compared with PTFs reported in the literature.

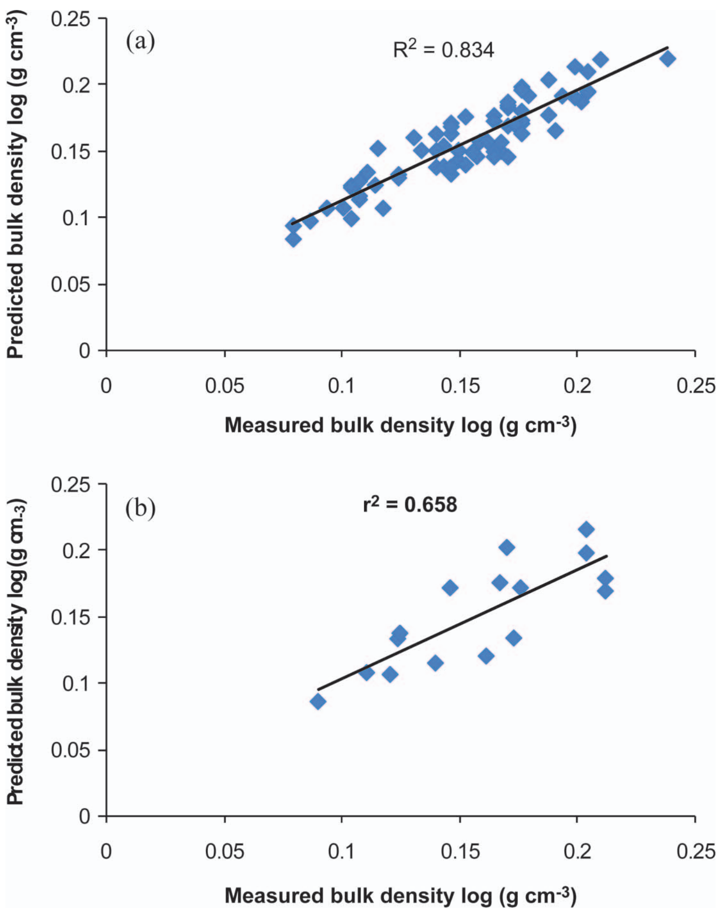

Figure 4. Correspondence between measured and predicted bulk density values with sand, silt fractions and moisture constants [field capacity (FC) and permanent wilting point (PWP)] data as an input in derived pedotransfer function (PTF): (a) training and (b) testing data set.

Compared with statistical regression, superiority of neural regression was evident from the evaluation indices for fitted data as well as test data. Neural regressions usually require at least three input variables to establish dependencies between the input and output. The input variables were always three or more in this study so it can be inferred that limitations of neural regression as a tool were addressed and it is the inadequacies of the data or insufficient spread of the data that caused poor network training. These shortcomings were overcome when information on physical structure as well as pore structure was related to BD. The study also suggests that PTFs could be successfully calibrated even for problem soils.

Conclusion

The study demonstrated that native PTFs to predict the BD of seasonally impounded soils could be calibrated successfully provided the correct choice of input variables is made. Further, it was also observed that statistical regression as a tool to establish dependencies between basic soil properties and BD had severe limitations and neural regression was a preferred method for calibrating PTFs. Contrary to expectations, the clay fraction was found to be an unimportant input parameter in predicting soil BD of the study soils. Owing to the narrow range of variation in organic carbon content, its influence on BD was not adequately expressed when neural networks were tested for predictive ability. However, there were indications that a greater spread of data or a greater quantity of data could alter the results. The best-performing PTF required input data on sand, silt, FC and PWP to predict BD, whereas the second best PTF required textural information, OC, FC and PWP as an input. Other PTFs using an intermediate number of input parameters performed poorly. The two proposed neural PTFs were shown to have reasonable predictive ability.

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