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Data compression by principal component analysis (PCA) in modelling of soil density parameters based on soil granulation

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The parameter for the density specification of naturally compacted non-cohesive soils and soils in embankments of hydraulic structures is the density index (I_D). The parameter used to control the quality of compaction of cohesive and non-cohesive soils artificially thickened, embedded in a variety of embankments is the degree of compaction (I_S). In order to determine the parameters of density (I_D or I_S), compaction parameters ($_{d\min}$, $_{d\max}$ or $_{ds}$, w_{opt}) should be examined in a laboratory, which often is a long and difficult procedure to carry out. Therefore, there is a need for methods of improving and shortening the test of compaction parameters based on the development and application of useful correlations. Since compaction parameters are dependent on the soil granulation, a method based on regression and artificial neural networks was applied to develop required correlations. Due to the large number of input variables of neural networks in relation to the number of case studies, a PCA method was used to reduce the number of input variables, which resulted in reduction in the size of neural networks.

Key words: artificial neural networks, principal component analysis, compaction parameters, minimum and maximum dry density of solid particles, graining parameters.

INTRODUCTION

The parameter for the density specification of naturally compacted non-cohesive soils and embankments of hydraulic structures is the density index (I_D). The parameter used to control the quality of compaction of cohesive and non-cohesive soils artificially thickened, embedded in a variety of embankments (communication tract embankments, earthen structures, backfills) is the degree of compaction (I_S).

Density index (I_D) also called a relative density (D_R) in literature (Lade et al., 1998) and the degree of compaction (I_S) are calculated according to the following formulas:

$$I_D = \frac{d_{\max}}{d} \cdot \frac{d - d_{\min}}{d_{\max} - d_{\min}} \quad [1]$$

where: $_{d\min}$, $_{d\max}$ – the minimum and maximum dry density of solid particles determined in the laboratory according to PN-88/B-04481 (1988) in the mould (height h = 12.54 cm and diameter D = 7.10 cm) using a vibrating fork simulating compacting of non-cohesive soil due to geological processes [Mg m^{-3}];

$$I_S = \frac{d}{d_{\max}} \cdot \frac{d}{d_s} \quad [2]$$

where: $_{d\max}$ – the maximum dry density of solid particles determined in the laboratory according to PN-88/B-04481 (1988) by the dynamic compaction method (the Standard Proctor test) which stimulates artificial compaction of soil by use of the compacting equipment [Mg m^{-3}]; $_{d\max}$is referred to as $_{ds}$ to avoid identifying this value as the maximum dry density of solid particles determined using a vibrating fork, thus $_{ds}$ is not equal to $_{d\max}$ in formula [1]; $_{ds}$ – thedry density of solid particles determined for soil in an embankment or in the ground [Mg m^{-3}].

Compactibility is the ability of the soil to achieve the dry density of the solid particles $_{ds}$, and it depends, among other things, on the physical characteristics of the soil: granulometric and lithologic composition, shape and degree of roundness of grains, soil origin, and applied energy of compaction, as well as on the method for the energy transfer and the soil moisture during compacting (Proctor, 1933; Pisarczyk, 1977; Barton et. al., 2001). Compaction parameters are: $_{d\min}$, $_{d\max}$, $_{ds}$, w_{opt}, and $_{d\max}$ $_{ds}$. Optimum water content w_{opt} is the moisture content at which compacted soil reaches the maximum dry density $_{ds}$.

Quick and efficient quality control of the resulting density is very important when compacting soil layers assembled into embankments. Laboratory tests of compaction parameters are laborious and time-consuming. Conducting such tests will cause breaks in the process of composing of the embankment. Therefore, new methods of reducing the time of testing these parameters are being sought. Ways of improving the methods to determine the parameters of compaction $_{ds}$ and w_{opt} the Proctor test are particularly interesting. This applies particularly to cohesive soils, for which the Proctor test is especially long and complicated. Numerous analyses were conducted to develop empirical dependence of $_{ds}$ and w_{opt} parameters on other geotechnical parameters, such as the Atterberg limits (liquid

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and plastic limits), plasticity index, granulation and compaction energy, using statistical models (Gurtug and Sridharan, 2004; Sivrikaya, 2008; Sivrikaya et al., 2008) and evolutionary polynomial regression, as well as artificial neural networks (Singha and Wang, 2008; Alavi et al., 2010; Ahangar-Asr, 2011). A review of these relationships was carried out in a number of articles, among others by Dąbska and Pisarczyk (2012), and Sulewska (2012).

The aim of this work is to continue searching the best relationship between the compaction parameters of non-cohesive soils and their particle size distribution using a simple linear regression models and nonlinear regression, multiple regression, artificial neural networks and principal component analysis (PCA).

DESCRIPTION AND RESULTS OF EXPERIMENTAL PROCEDURES

Laboratory tests were carried out on 121 samples of Pleistocene non-cohesive soils originating from the Odra Glaciation, in the area around the city of Białystok. The samples were the natural soils or specially screened off from the natural soils to obtain a diversified grain: silty sands (code 1), fine sands (code 2), medium sands (code 3), coarse sands (code 4), sand and gravel mixes (code 5) and gravels (code 6; Sulewska, 2010a, b). For each soil sample, the studies of compaction parameters and grain-size analysis were conducted complying with PN-88/B-04481 (1988). On the basis of grain-size distribution, curve grain diameters D_x were defined below which x% of soil mass is placed, for x = 10, 20, ..., 90, and uniformity coefficient C_U:

$$C_U \quad \frac{D_{60}}{D_{10}} \qquad [3]$$

The value ranges for the parameters are shown in Table 1.

Figure 1 supports the view that the compaction parameters are influenced by the type of soil (i.e. grain size). It can be observed that along with increasing grain size $_{d\min}$, $_{d\max}$, $_{ds}$, values also grow, whereas w_{opt} values decrease.

Table 1

The geotechnical parameters of tested soils

Soil code	1–6
$_{d\min}$ [Mg m^{-3}]	1.247–1.881
$_{d\max}$ [Mg m^{-3}]	1.604–2.124
$_{ds}$ [Mg m^{-3}]	1.587–2.200
w_{opt} [%]	2.1–17.7
C_U [–]	1.25–12.50
D_{10} [mm]	0.019–0.500
D_{20} [mm]	0.040–1.00
D_{30} [mm]	0.040–2.20
D_{40} [mm]	0.060–2.85
D_{50} [mm]	0.070–3.50
D_{60} [mm]	0.084–4.50
D_{70} [mm]	0.093–6.00
D_{80} [mm]	0.110–10.00
D_{90} [mm]	0.140–25.00

STATISTICAL ANALYSIS OF TEST FINDINGS

Statistical analysis of the results of tests was carried out using *STATISTICA* software (Stanisz, 2007). Models of linear, curvilinear and multiple regression (Sulewska, 2010a, b) are shown in Table 2.

Interdependencies between variables were preliminarily analysed on the basis of linear correlation matrix and it was found that there were statistically significant linear correlations between the parameters of compaction ($_{d\min}$, $_{d\max}$, $_{ds}$, w_{opt}) and the parameters of particle size (C_U, D_{10}–D_{90}), at determination coefficient R^2 = 0.31–0.76. Moreover, it was not possible

Table 2

Models of linear, curvilinear and multiple regression

Model	Formula	Determination coefficient R^2	Formula number
$_{d\min}$			
Linear correlation	$_{d\min} = 1.380 + 0.038C_U \pm 0.110$	0.34	[4]
Curvilinear correlation	$_{d\min} = 1.364 + 0.139\ln C_U \pm 0.113$	0.31	[5]
Multiple regression	$_{d\min} = 1.322 + 0.018C_U + 0.734D_{10} \pm 0.091$	0.55	[6]
$_{d\max}$			
Linear correlation	$_{d\max} = 1.676 + 0.040C_U \pm 0.082$	0.51	[7]
Curvilinear correlation	$_{d\max} = 1.655 + 0.152\ln C_U \pm 0.084$	0.49	[8]
Multiple regression	$_{d\max} = 1.637 + 0.027C_U + 0.499D_{10} \pm 0.071$	0.64	[9]
$_{ds}$			
Linear correlation	$_{ds} = 1.589 + 0.060C_U \pm 0.078$	0.72	[10]
Curvilinear correlation	$_{ds} = 1.551 + 0.235\ln C_U \pm 0.076$	0.73	[11]
Multiple regression	$_{ds} = 1.619 + 0.035C_U - 0.100D_{50} \pm 0.070$	0.78	[12]
w_{opt}			
Linear correlation	$w_{opt} = 14.8 - C_U \pm 2.3$	0.46	[13]
Curvilinear correlation	$w_{opt} = 15.6 - 4.1\ln C_U \pm 2.3$	0.49	[14]
Multiple regression	$w_{opt} = 15.9 \quad 0.7C_U - 13.5D_{10} \pm 2.00$	0.59	[15]

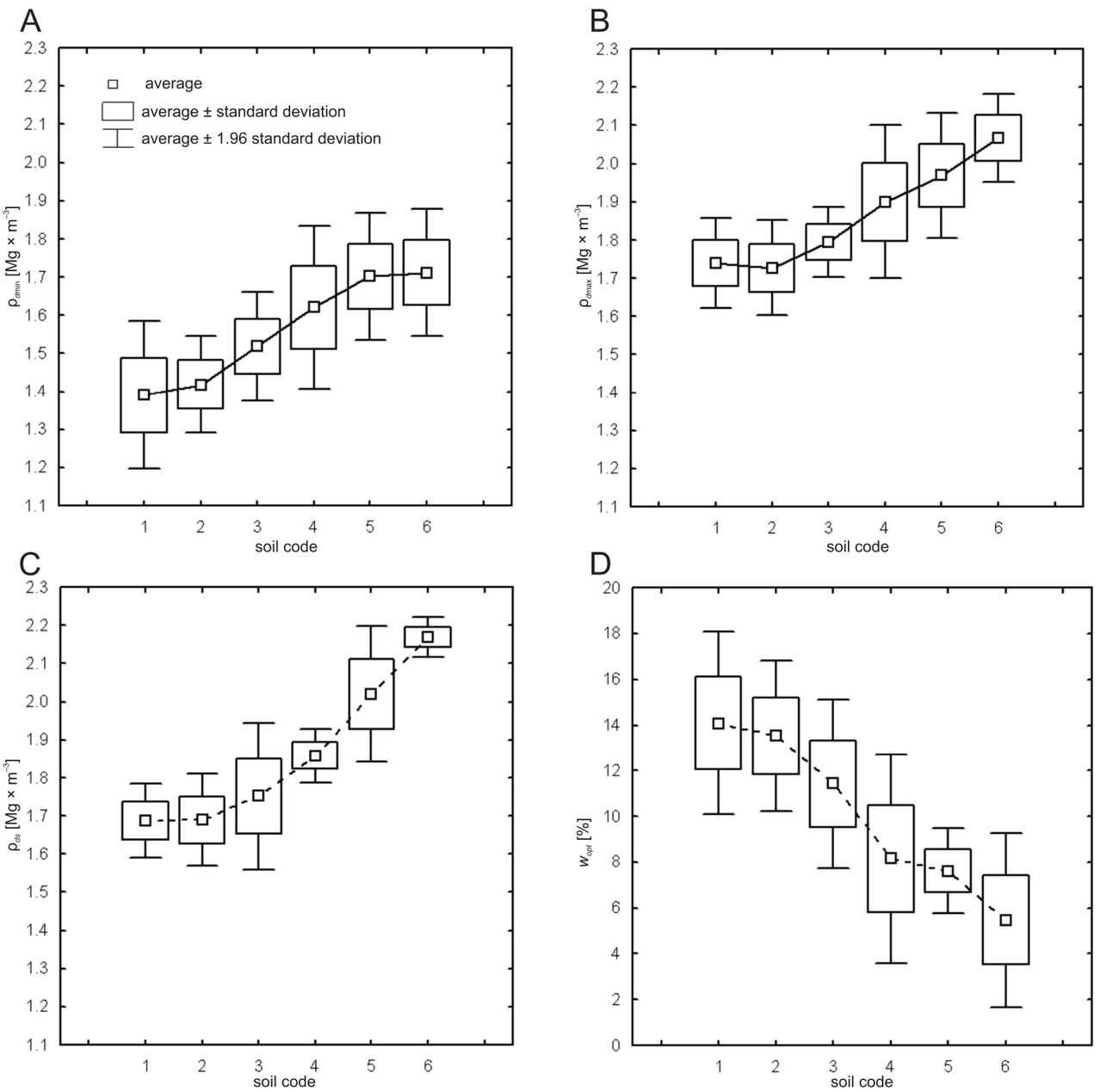

Fig. 1. Average values of compaction parameters for groups of soils 1–6

A – $_{dmin}$; **B** – $_{dmax}$; **C** – $_{ds}$; **D** – w_{opt}

to distinguish any particular grain diameters as the most influential ones –- all diameters D_x affect the analysed parameters to a similar extent. Correlations between w_{opt} and diameters D_x are negative, whereas those between $_{dmin}$, $_{dmax}$, $_{ds}$ and diameters D_x – are positive. All parameters of the grain are mutually highly correlative – the coefficient of determination of interdependence between the different parameters of the particle size is R^2 = 0.30–0.98 (Sulewska, 2010b).

It can be seen that the multiple regression models are better than linear and nonlinear models with one explanatory variable, because they have a higher R^2. However, they are not very good quality models and explain only from 55 to 64% of the observed variation (when R^2 = 0.55–0.64), with the exception of the $_{ds}$ models which explained about 72–78% of the variation. It should be noted that the multiple regression models included only a few variables: C_U and D_{10} or D_{50}. Other explanatory variables entered into the multiple regression models proved to be statistically insignificant. This situation is the result of alignment of the variables. The variables describing the particle size distribution are mutually strongly correlated. Therefore, the obtained determination coefficients do not reflect the full impact of the independent variables on the dependent one, expressing it only partially (Stanisz, 2007). In order to account for the effects of all parameters of particle size on the analysed compaction parameters, the artificial neural networks were applied as they do not have to conform to a number of theoretical assumptions and are not subject to the limitations of statistical analysis of data

(e.g., concerning normal distribution of variables or cross-correlation between the independent variables).

ARTIFICIAL NEURAL NETWORKS (ANNs)

Artificial neural networks (ANNs) function on the principle of the parallel operation of neurons. Each neuron is a single transducer of signals (Haykin, 1999; Osowski, 2006). To solve regression problems, the most commonly used types of networks are multi-feed-forward layered networks MLP (Multi-Layered Perceptrons). They consist of a number of input variables, one or more hidden layers and the output layer of one or more outputs M (output variables). For example, identification of neural network architecture: 10-4-1 represents a network with 10 inputs, 4 neurons in the hidden layer and one output.

A feed-forward operation of the network consists in processing the input signal $x^{(p)}$ into the output signals $y^{(p)}$ (Waszczyszyn, 1999):

$$x^{(p)}_{(Nx1)} \quad y^{(p)}_{(Mx1)} \tag{16}$$

Input and output vectors have the following components:

$$x^{(p)}_{(Nx1)} \quad x_1,\ldots,x_N{}^{(p)}, y^{(p)}_{(Mx1)} \quad y_1,\ldots,y_M{}^{(p)} \tag{17}$$

To learn and test networks, a set of P patterns, i.e. pairs of input/output vectors of known components are used:

$$P \quad x,y^{(p)};p \quad 1,\ldots,P \tag{18}$$

The set P is randomly split into subsets: the learner L and T test:

$$L \quad x,y^{(p)};p \quad 1,\ldots,L \quad ,T \quad x,y^{(p)};p \quad 1,\ldots,T \tag{19}$$

where: L – number of learner patterns, T – number of test patterns, P – numbers of patterns.

The aim of the network learning process is to adjust network parameters, i.e. a set of weights and trigger points (bias) allowing to obtain possibly the smallest approximation error, i.e. the smallest difference between the approximated element $d_i^{(p)}$ and the approximating element $y_i^{(p)}$. After entering signals $x^{(p)}$ into the network, instead of the expected response $d^{(p)}$, the output vector $y^{(p)}$ is obtained, with the accuracy equal to the required values $d_i^{(p)}$. Learning network is minimizing the error function, which can be calculated for the entire network as the mean square error for the set P:

$$E \quad \frac{1}{2}\sum_{p\ 1}^{P}\sum_{i\ 1}^{M} d_i^{(p)} \quad y_i^{(p)}{}^{2} \tag{20}$$

where: M – number of outputs, i – output number, $i = 1, \ldots, M$.

Learning algorithms are iterative. In each epoch, all the cases from the training set are introduced to the network and followed by improvement of network weights. Selection of optimal network design is done in an empirical way. In order to establish artificial neural network's architecture, the number of hidden layers and the number of neurons in each hidden layer must be specified.

The main feature of neural network is the ability to generalize the acquired knowledge. In order to achieve good generalization of the network, it is necessary to minimize network structure, as well as to train it on a sufficiently large set of training data. The larger the ratio of the number of learning patterns L to the number of network parameters NNP, the better the generalization properties of the network. It is difficult, however, to give recommendations for the above ratio. For example, in the work by Waszczyszyn (1999), it is recommended that the following condition was met:

$$NNP \quad L \quad M \tag{21}$$

In this paper, the feed-forward neural network with one hidden layer and one output were exercised. Multilayer feed-forward networks with one hidden layer were applied to solve the analysed regression problems. For such networks, the number of network parameters (NNP) is calculated according to the formula:

$$NNP \quad N \quad H \quad H \quad M \quad H \quad M \tag{22}$$

where: N – number of inputs, H – number of neurons in a hidden layer, number of outputs $M = 1$.

The greater the number of neurons in the network (i.e. NNP), the greater the number of training data it should be provided with. Reducing the NNP can be done, among other methods, by linear transformation of the dimension of data space into a space of a smaller size through principal component analysis (PCA; Haykin, 1999; Osowski, 2006; Stanisz, 2007).

NEURAL MODELS

The neural analyses were conducted using the *STATISTICA Neural Networks PL* software, where cases are randomly assigned to the subsets: L – learning subset, V – validation subset (which is used to independently verify the quality of the network during the learning process) and T – testing subset (which carries out a one-off calculation of network error at the end of learning). The accepted ratio is 50:25:25% of the total patterns, i.e. 61:30:30 patterns, respectively. The most effective training method was the Variable Metric Method with algorithm of the Broyden-Fletcher-Goldfarb-Shanno (BFGS) in this study (Osowski, 2006). The tanh sigmoid activation functions were applied in neurons of the hidden layers and linear functions in neurons of output layers. The best neural models of analysed compaction parameters are given in Table 4, further in the article. As input variables, all grain-size parameters were introduced (C_U, D_{10}–D_{90}). As error measures of ANN, the values of coefficient of determination R^2 and Mean Absolute Error (MAE) in the collections of L, V, T were applied, and the values of error measurements in the subset T were decisive:

$$R^2 \quad 1 \quad \frac{\sum_{p\ 1}^{P} d^{(p)} \quad y^{(p)}{}^{2}}{\sum_{p\ 1}^{P} d^{(p)} \quad \bar{d}^{(p)}{}^{2}} \tag{23}$$

$$MAE \quad \frac{1}{P}\sum_{p\ 1}^{P}\left|d^{(p)} \quad y^{(p)}\right| \tag{24}$$

where: $d^{(p)}$ – actual value, $y^{(p)}$ – predicted value of y, $\bar{d}^{(p)}$ – mean of the $d^{(p)}$ values.

PRINCIPAL COMPONENT ANALYSIS (PCA)

Principal component analysis (PCA) is a statistical procedure by which the initial variable X_j are transformed into mutually orthogonal PC_j new variables. By using PCA, the number of variables is reduced while maintaining the variability in the data as much as possible. If the initial variables are correlated, the knowledge of only a part of them is sufficient to determine other variables. This is done by creating new variables that are linear combination of the initial variables. The new variables are called principal components PC_j. The equation in the method of PCA is represented by a change, which is a special case of linear transformation according to the formula:

$$PC = Ax \qquad [25]$$

where: x – original variables vector, $x \quad R^N$, PC – principal components vector, A – matrix of coefficients, $A \quad R^{NxK}$, $K < N$.

Principal component analysis is the description of the process of transformation of an N-element vector x into a K-element vector PC via the matrix $A \quad R^{NxK}$. As the further analysis includes selected elements K, where $K < N$, the PCA transformation becomes a lossy compression. The K-element vector PC is a vector of principal components that have the greatest impact on the reconstruction of N-element data vector x. New variables (principal components PC_j) are orthogonal to each other, i.e. are uncorrelated. The principle of the PCA method is to ensure such a rotation of the coordinate system XOY so that the new $PC1OPC2$ axes coincide with the axes of the cloud of points in a scatterplot. The position of $PC1$ axis is planned so that it becomes an axis of the point cloud in the XOY system (Fig. 2).

The first principal component $PC1$ determines the direction in multidimensional space, with the maximum data variance. It explains most of the variance of the original variables. The variance of the main principal component $PC1$ is equal to the value of its eigenvalue $_1$ (Var($PC1$) = $_1$). Other main components explain the remaining, smaller and smaller proportion of the variance of the original variables (Var (PC_j) = $_j$).

Data compression was conducted to reduce the size of the neural network. Principal component analysis was used to create a new input variables on the basis of ten parameters describing the grain size of the soils (D_{10}–D_{90}, C_U), based on the correlation matrix between these parameters (Stanisz, 2007).

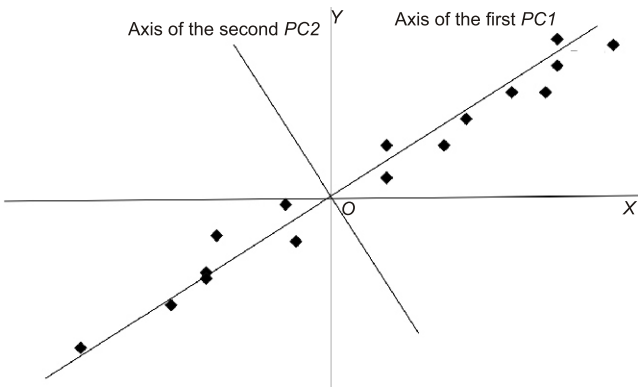

Fig. 2. Rotation of coordinate system in two-dimensional space (see Kuźniar and Waszczyszyn, 2006; Stanisz, 2007)

Table 3

Analysis of principal components

Principal components	Eigen value	Percent of total variance [%]	Cumulative percent of variance [%]
PC1	8.606	86.06	86.06
PC2	0.743	7.43	93.49
PC3	0.394	3.94	97.43
PC4	0.144	1.44	98.87
PC5	0.073	0.73	99.60
PC6	0.022	0.22	99.82
PC7	0.010	0.10	99.92
PC8	0.005	0.05	99.97
PC9	0.002	0.02	99.99
PC10	0.001	0.01	100.00

Table 3 presents the percentage of variance that is explained by each of the principal components. The first principal component $PC1$ accounts for 86.06% of the total variance, the second $PC2$ principal component accounts for 7.43% of the total variance.

According to the Kaiser criterion, only those main components are used whose main values are $_j > 1$ (in: Stanisz, 2007). It has been decided, however, to take into account the Cattell scree test (in: Stanisz, 2007) and the adoption of two principal components $PC1$ and $PC2$, which altogether explained 93.49% of the variance (Fig. 3). Principal components $PC1$ and $PC2$ will function as inputs of newly designed neural networks.

The PCA method was also used for the input data of data compression pre-processing.

NEURAL MODELS WITH APPLIED PCA

The best new artificial neural networks with two inputs ($PC1$ and $PC2$), one hidden layer and a single output are designated as ANN(PCA) and are presented in Table 4. ANN(PCA)s of

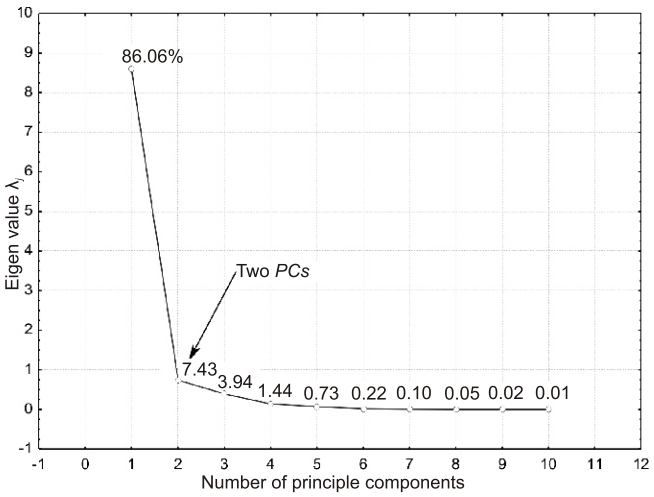

Fig. 3. Percentage of variance explained by following *PCs* and Catell's criterion

Table 4

ANNs and ANN(PCA)s with the best prediction accuracy and their error measures

Output – parameter	Architecture of ANN (training number of epochs)	*NNP*	*MAE*			R^2		
			L	*V*	*T*	*L*	*V*	*T*
ANNs								
d_{min}	10-4-1 (43)	49	0.050	0.052	0.065	0.73	0.65	0.82
d_{max}	10-4-1 (134)	49	0.040	0.055	0.047	0.74	0.71	0.70
d_s	10-4-1 (28)	49	0.038	0.035	0.050	0.87	0.89	0.87
w_{opt}	10-4-1 (48)	49	1.02	1.49	1.88	0.76	0.67	0.67
ANN(PCA)s								
d_{min}	2-6-1 (37)	25	0.058	0.056	0.066	0.67	0.72	0.72
d_{max}	2-6-1 (201)	25	0.047	0.052	0.050	0.73	0.65	0.67
d_s	2-6-1 (516)	25	0.034	0.038	0.045	0.89	0.89	0.89
w_{opt}	2-6-1 (325)	25	1.34	1.34	1.11	0.72	0.71	0.72

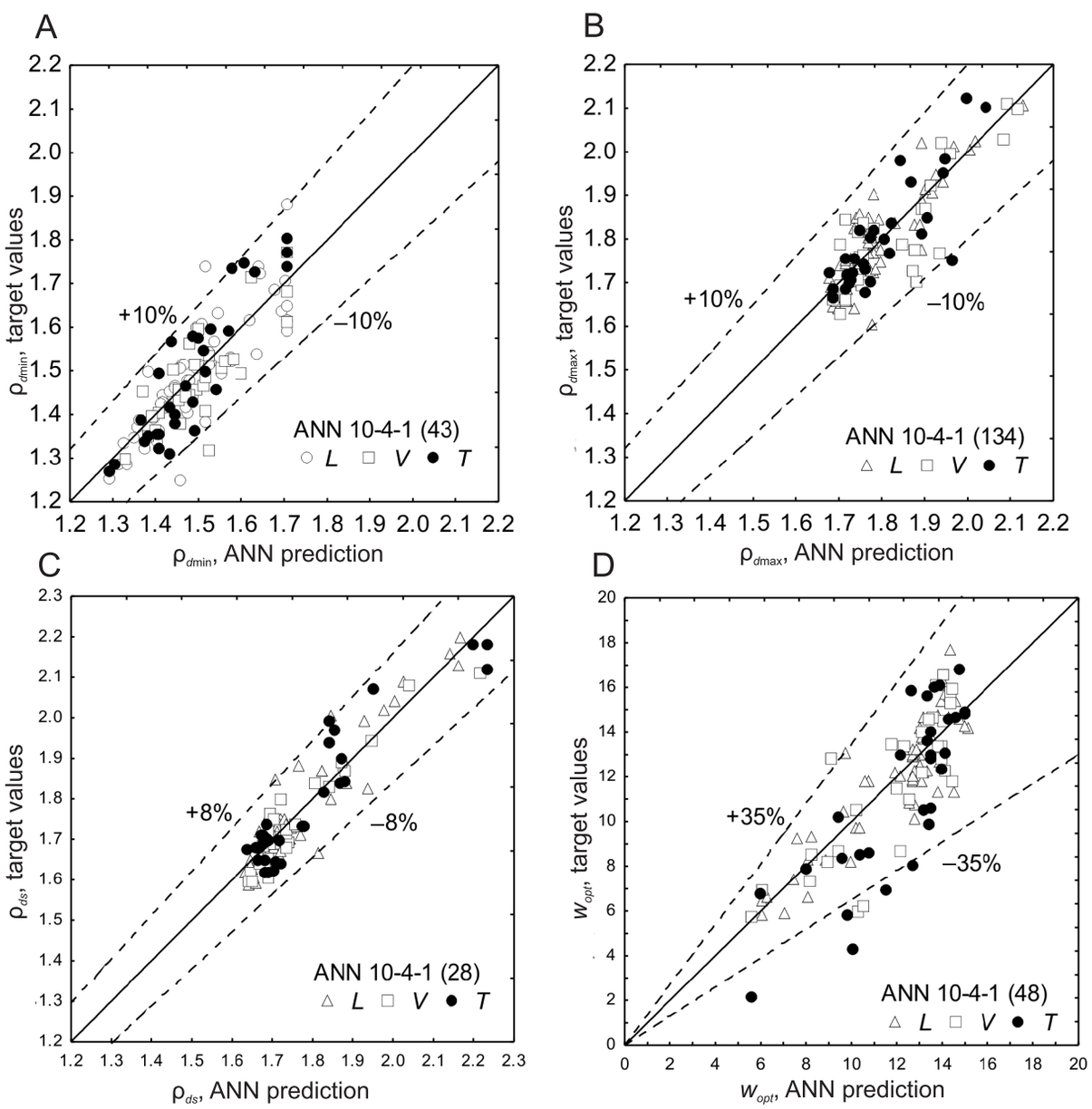

Fig. 4. Comparison between target values and predicted values by ANNs

A – d_{min}; **B** – d_{max}; **C** – d_s; **D** – w_{opt}; other explanations as in Table 4

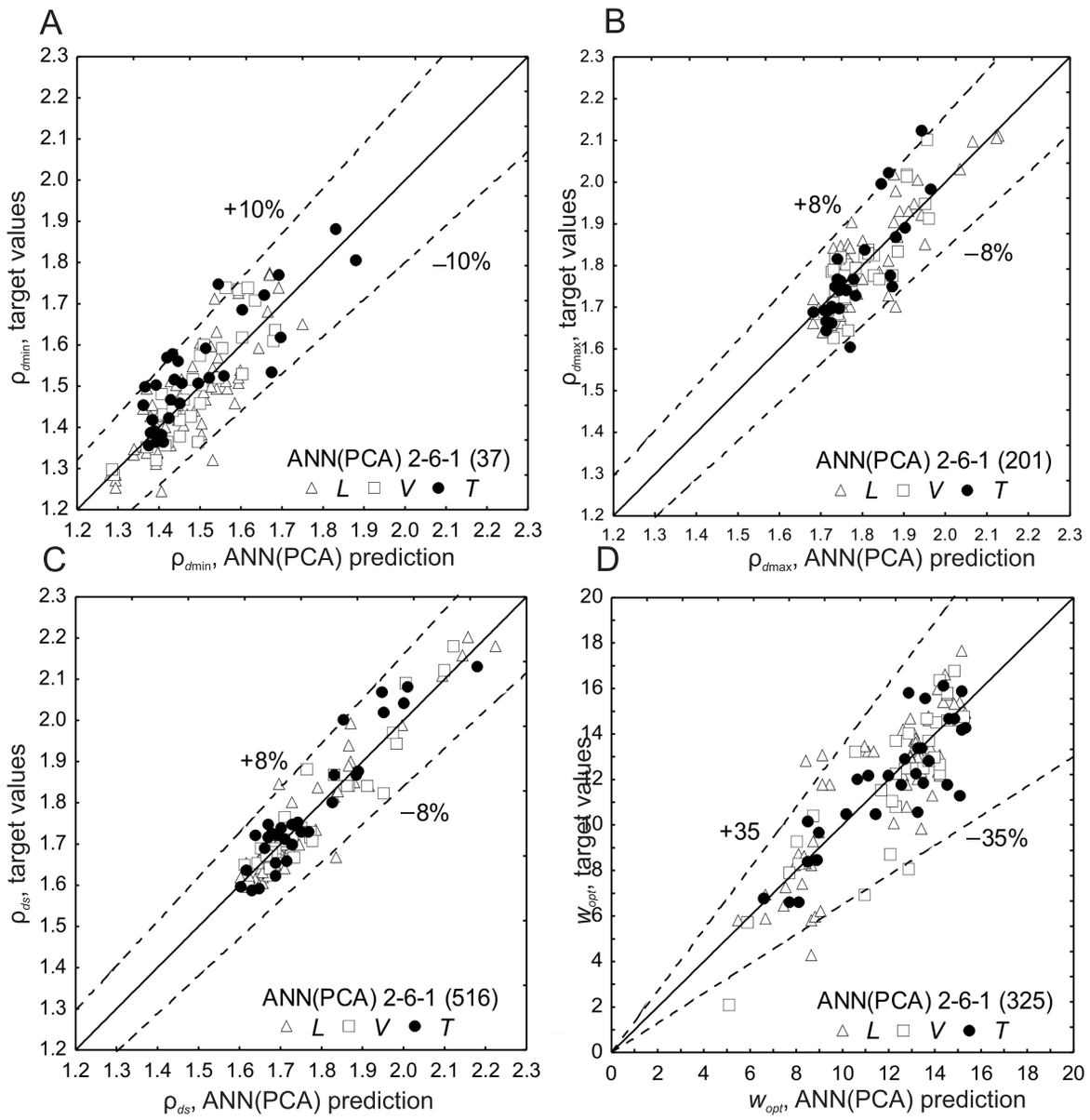

Fig. 5. Comparison between target values and predicted values by ANN(PCA)s

A – $_{dmin}$; **B** – $_{dmax}$; **C** – $_{ds}$; **D** – w_{opt}; explanations as in Table 4

comparable predictive quality were obtained when using 3 inputs (*PC1–PC3*) or 4 inputs (*PC1–PC4*) as well as 2 inputs (*PC1* and *PC2*). The third (*PC3*) and/or fourth (*PC4*) principal components (variables) were not often included in the model as a result of resetting the weights.

In conclusion of the analysis of networks, summarized in Table 4, it can be stated that the quality of prediction of compaction parameters $_{dmin}$, $_{dmax}$, w_{opt} and $_{ds}$ is quite good, and by applying the neural networks, the most accurately predicted parameter was $_{ds}$. Comparison of neural network quality measures contained in Table 4 shows that the PCA method of data compression enabled the construction of neural networks ANN(PCA)s with a much smaller number of neurons, and a smaller number of network parameters than ANNs. In contrast, after analysing the measurements of errors *MAE* and R^2, it can be concluded that the accuracy of predictions did not decrease or decreased only to a small extent. Figures 4 and 5 show the relative error (*RE*) of prediction by using ANN and ANN(PCA) models, calculated according to the formula:

$$RE \left| \frac{y^{(p)} \quad d^{(p)}}{y^{(p)}} \right| 100\% \qquad [26]$$

RESULTS AND CONCLUSIONS

Comparing the values of the coefficient of determination in regression models shown in Table 2 and neural models shown in Table 4, it can be concluded that, in general, neural models (R^2 = 0.67–0.89 in the test subset) have a better predictive value than the regression models (R^2 = 0.31–0.78). Considering the ANNs and ANN(PCA)s models (Table 4), it can be stated that compression of input data by the PCA method and

reducing the number of input data to the neural networks (from 10 variables to 2 variables) resulted not only in reducing the number of neural network parameters (from 49 to 25), but also in improving the prediction accuracy for $_{ds}$ and w_{opt}. The smallest improvement in predictive quality was obtained for parameter $_{d\max}$, whereas the greatest improvement in the quality of prediction was obtained by using a neural network for the parameter $_{d\min}$ (R^2 = 0.82 and R^2 = 0.72 for the test subset). The clearest correlations can be observed between soil particle size distribution and maximum bulk density of soil matrix through the Proctor test method $_{ds}$. The ANN model (PCA) reached a value of R^2 = 0.89 in the test subset. Kłos et al. (2011) reports that it was possible for modelling of $_{ds}$ by means of semi-Bayesian Neural Network (SBNN) with pre-processing of input data using PCA (array covariance matrix) for the SBNN PCA model 10-2-1 to obtain value R^2 = 0.93 for the test subset. Application of PCA in modelling the compaction curves of fly ash using ANNs has also produced very good results and allowed obtaining a neural network of satisfactory accuracy (Zabielska-Adamska and Sulewska, 2012). It can be concluded that the ANN tool can be used to analyse the results of experimental studies and to obtain the relationships between the test values with a better accuracy than by the regression method, which, however, has the advantage of an explicit character of the pattern.

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