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APPLICATION OF TWO-PHASE REGRESSION TO GEOTECHNICAL DATA

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A method for estimating a transition parameter in two-phase regression is described. The two phases are fitted and simultaneously the transition point is estimated. Practical application of the method is demonstrated on the data for determining soil hydraulic properties.

1. Introduction

The method of two-phase regression needs to be used when the dependent variable behaves differently in two intervals of the independent variable. Situations where data (original or transformed) behave according to two or more different straight line relationships are examined in many applications. It is known sometimes prior to the experiment, that in the studied material, for example a structural change occurs, when the independent variable exceed a given threshold.

The function of a two-phase regression may be presented as

$$f(X;\alpha,\beta,\gamma) = \begin{cases} f_1(X;\alpha), & X < \gamma \\ f_2(X;\beta), & X \geq \gamma, \end{cases} \tag{1}$$

where γ is a transition point while functions f_1 and f_2 depend on the unknown parameter vectors α and β. To ensure continuity of the function (1) the following condition has to be satisfied: $f_1(\gamma;\alpha) = f_2(\gamma;\beta)$.

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In literature there are methods of determining a multi-phase linear regression with known and unknown transition point [11], [3], [13]. The situation is relatively simple when the threshold value (transition point), is known. However, it is rarely the case of geotechnical data which is the subject of the present work.

In geotechnics, wetting fluid saturation in a porous media during drainage cycle typically decreases with suction increase. The soil water characteristic curve (SWCC) relates matric suction, ψ, or water pressure head, h to the water content (i.e., either volumetric θ or gravimetric) or degree of saturation (see for example [9]). The true relationship is basically unknown. The shape of the curve is usually observed by experimental measurements for each particular soil. The features of the SWCC are the volumetric water content at saturated condition, θ_s, the residual water content and the air-entry/expulsion value. The air-entry value, *aev* of the soil is the matric suction value where air enters into the soil pores. Other definitions without stated physical meaning are also present in the literature. Widely used in the soil mechanics literature is the geometrical definition of the *aev* using a tangent to the fitted SWCC in its second phase.

Scientific knowledge of the desiccation process in soils indicates that if there is no volume change then the volumetric water content, θ, will stay almost constant for matric suction, ψ, up to the air entry value. This constant characterizes the volumetric water content at saturated condition. For suction greater than the *aev* the volumetric water content will decrease rapidly at first, but then level off as the drying progresses. In theory the volumetric soil water content will actually reach 0 when the water is fully removed from the soil. However, a full removal is unlikely in reality, because there is always some water remaining in the pores that leaves the soil more and more slowly. As a result, the process will approach only asymptotically some residual water content. Further pressure increase may cause soil deformation rather than water removal. Although the residual water content does not correspond consistently to a recognized physical entity, we assume that after this point the water removal behaves differently. In this paper we are not interested in the process beyond this point since no much data is possible to be obtained and therefore to be used in statistical modeling. Note that the popular Brooks–Corey relationship [5] is also not recommended for saturation less than residual water content [6]. There are however approaches in which the SWCC is defined as a single curve [7], [8] and therefore no changes of the process behaviour is assumed in such models. Consequently, model equations do not include *aev* as a parameter.

In this paper, we consider a two-phase regression model of the SWCC with unknown transition point. This extra parameter has to be estimated based on the process observations. Appropriate data transformations are used in order to meet the regression assumptions and to make the regression linear. The modified least squares method gives a solution by minimizing the residual sum of squares with respect to the regression parameters as well as transition point parameter. The procedure uses methods known earlier which, however, are significantly modified to be appropriate for soil data. The approach is illustrated on a data set for sand soil taken from the literature.

2. Model assumptions

The soil data for SWCC measurements is well recognized as at least two-phase problem for the regression analysis. There are two more special features of the SWCC data. The first one is that measurement of the water content is not equally precise along the full matric suction range. One can observe that θ measurement is more precise for small values and less precise for large values of ψ [14], [1]. Therefore a multiplicative error is more proper to be used. The distribution of the error hereafter is assumed Log-normal. Second feature of the soil measurement is that the regression of θ on ψ is nonlinear on the second phase for any type of soil. Dealing with these problems is usually done by appropriate data transformations [12], [4].

Let Y and X denote some transformations of θ and ψ, respectively, that force data to meet the assumption for constant variation of Y at each X. Some of these transformations also cause a linear dependence of Y on X in the second phase. Useful transformations of SWCC data that represent data as a linear pattern are discussed in [15].

Applying appropriate transformation the regression of Y on X is represented by two intersecting straight lines, one being appropriate when ψ takes values below and the other when ψ takes values above the air entry value.

In this paper we are assuming that:

1. Within each phase the observed Y values are normally distributed with mean zero and constant standard deviation about the true regression line (classical regression assumption);

2. The transition occurs in some known interval, but it is not known exactly between which two observed X values it takes place.

The value of the saturated water content which gives us the first phase line is considered both unknown (Section 3.1.) and known (Section 3.2.).

A difficulty arises if against the assumption 2 the intersection of the fitted lines has an X coordinate falling outside the estimated interval for the transition point. The experimenter must then decide whether to attribute this to sample errors, or an incorrect assumption about the location of the transition point, and determine the appropriate procedure accordingly.

3. Two-phase linear model of the SWCC

Let (ψ_i, θ_i), $i = 1, \ldots, n$, be n pairs of observations of matric suction and volumetric water content, respectively. Let (X_i, Y_i) be the set of the transformed observations of θ and ψ, which make data to follow linear relationship. Here X_i corresponds to the i-th observation of the matric suction, ψ_i, and Y_i corresponds to the observed volumetric water content at ψ_i. The independent observations $X_1 \ldots, X_n$ are assumed ordered and the measurement errors are uncorrelated $N(0, \sigma^2)$.

The regression function of a two-phase SWCC can be presented by

$$Y = \begin{cases} \tau, & X < \gamma \\ \beta_0 + \beta_1 X, & X \geq \gamma, \end{cases} \tag{2}$$

where $\beta = (\beta_0, \beta_1)$ is the set of the *unknown* regression parameters of the second phase, γ is the *unknown* transition point, and τ corresponds to the *unknown* saturated volumetric water content. Here the parameter γ is the transformed value of the *aev* by the same transformation applied to ψ, while τ is the transformed value of the saturated volumetric water content by the same transformation applied to θ.

The transition point satisfies the linear constraint

$$\beta_0 + \beta_1 \gamma = \tau \tag{3}$$

to ensure the continuity of the solution in transition point.

Modeling a given phenomenon with two-phase linear regression consists in estimating unknown parameters (in our case $\beta = (\beta_0, \beta_1)$, τ and γ), based on the observations. The independence, homoscedasticity, and normality of the errors allow the use of an extension of ordinary least sum of squares regression method for estimating the model parameters.

Adapting the least squares method, it is possible to gain estimates of α, β and γ (if the last one is unknown), which minimize the sum

$$S^2(\tau, \beta, \gamma) = \sum_{X_i < \gamma} (Y_i - \tau)^2 + \sum_{X_i \geq \gamma} (Y_i - \beta_0 - \beta_1 X_i)^2, \tag{4}$$

subject to (3). We allow not less then two observations in each phase in order to proceed the minimization.

The emphasis in this paper is on estimating and making inference about the transition parameter γ.

3.1. Estimating the air-entry value

Let us consider the model (2). If the transition point is known, the minimum of $S^2(\tau,\beta,\gamma)$ can be found minimizing each component of (4) separately, based on a properly determined sets of observations. This, however, does not ensure the continuity of the solution (3) in the transition point. We apply different approach dealing with this problem.

For each β and τ fixed, $S^2(\tau,\beta,\gamma)$ as a function of γ changes only when the transition point parameter γ passes over the sample points X_t of the independent variable X. Therefore conditional on $X_t < \gamma \le X_{t+1}$, the residual sum of squares $S^2(\tau,\beta,\gamma)$ can be minimized over τ and β, and this yields a sequence of residual sums of squares functions $S_t^2(\tau,\beta,\gamma)$ ($t = 3,\dots,n-2$, and $X_t < \gamma \le X_{t+1}$). The sequence of functions $S_t^2(\tau,\beta,\gamma)$ is segmenting overall $S^2(\tau,\beta,\gamma)$. That is

$$S^2(\tau,\beta,\gamma) = S_t^2(\tau,\beta,\gamma) \quad \text{if} \quad X_t < \gamma \le X_{t+1},\ t = 3,\dots,n-2 \tag{5}$$

where by definition

$$S_t^2(\tau,\beta,\gamma) = \sum_{i=1}^{t-1}(Y_i-\tau)^2 + \sum_{i=t}^{n}(Y_i-\beta_0-\beta_1 X_i)^2. \tag{6}$$

Therefore, the minimization of $S^2(\tau,\beta,\gamma)$ can be done over the function (6) as follows. The first stage is to compute the minimum of $S_t^2(\tau,\beta,\gamma)$ with respect to τ and β for $t = 3,\dots,n-2$. Denote $\hat\tau(t)$ and $\hat\beta(t)$ the minimizers for τ and β when $X_t < \gamma \le X_{t+1}$.

In the second stage, we compute the estimator of γ using the linear constraint for the two phases (3):

$$\hat\gamma(t) = \frac{\hat\tau(t)-\hat\beta_0(t)}{\hat\beta_1(t)}.$$

Now since $S_t^2(\tau,\beta,\gamma)$ corresponds to $S^2(\tau,\beta,\gamma)$ only for $X_t < \gamma \le X_{t+1}$, it follows that either

$$\hat\gamma = \hat\gamma(t) \ \text{ for some } t, \text{ in case } X_t < \hat\gamma(t) \le X_{t+1},$$

or

$$\hat\gamma \ne \hat\gamma(t) \ \text{ for some } t, \text{ in case } \hat\gamma(t) \text{ lies outside the interval } (X_t, X_{t+1}).$$

To determine $\hat\gamma$ we have to compare the values of $S_t^2(\hat\tau(t),\hat\beta(t),\hat\gamma(t))$ for all t such that $X_t \le \hat\gamma(t) < X_{t+1}$ and choose t^* which gives the minimum value for S_t^2.

If for some t the intersection of the fitted lines, $\hat{\gamma}(t)$ is falling outside the assumed interval $[X_t; X_{t+1})$, one should use the confidence interval to decide whether to attribute this to sample errors or an incorrect assumption. In such case Hinkley, [10] proposed to use $\hat{\gamma} = X_t$ or $\hat{\gamma} = X_{t+1}$ depending on S^2. However, the observations X_t or X_{t+1} may have a large measurement error and this error will be included in the estimation of τ. In our case of constant first phase, this method gives $\tau = Y_t$ or $\tau = Y_{t+1}$, which is obviously not applicable.

The transition point estimate $\hat{\gamma}$ separates observations into two phases. Thus the first phase observations are used to estimate τ while the second phase observations are used to estimate β_0 and β_1. For *known* transition point these estimates coincide with ordinary least squares estimates obtained by two regression lines passing trough the fixed point, namely the transition point.

Confidence interval for γ. Since $\hat{\gamma}$ is a ratio of two correlated normal random variables, $\hat{\tau} - \hat{\beta}_0$ and $\hat{\beta}_1$, we use Fieller's method to find an interval estimate for γ.

The $100(1-\alpha)$ confidence interval for γ is obtained by the solutions of

$$[\hat{\tau} - \hat{\beta}_0 + \hat{\gamma}\hat{\beta}_1]^2 - \frac{n_1 n_2}{n} F^{\alpha}_{1,n-3} \frac{S^2}{n-3} = 0, \tag{7}$$

where $\hat{\tau}$, $\hat{\beta}_0$, $\hat{\beta}_1$ and $\hat{\gamma}$ are the estimated parameters, S^2 is the residual sum of squares 4 for these estimates, $F^{\alpha}_{1,n-3}$ is the upper α critical value for the F-distribution with 1 and $n-3$ degrees of freedom, and n_1 and n_2 are the number of observations in the first and the second phase, respectively.

3.2. Modification for known saturated volumetric water content

Now suppose that the saturated volumetric water content, θ_s, respectively τ is known. We suppose that data satisfy the linear regression assumptions for the model (2). The parameters $\beta = (\beta_0, \beta_1)$ and γ are assumed unknown and should be estimated through the data.

The function to be minimize is simplified by eliminating the first term in (4) and in this case we have:

$$S^2(\beta, \gamma) = \sum_{X_i \geq \gamma} (Y_i - \beta_0 - \beta_1 X_i)^2, \tag{8}$$

subject to $\beta_0 + \beta_1\gamma = \tau$.

If the transition point is known, the minimum of $S^2(\beta, \gamma)$ can be found using only the observations after this point. The rest of the data should be viewed as error measurement of the saturated volumetric water content. Such an approach is used in [5] and [6] for $X = \log\psi$ and $Y = \log\theta$ for data after air entry value.

Conditional on $\gamma \geq X_t$, $S^2(\beta,\gamma)$ is minimized over β. Denote $\hat{\beta}(t)$ the minimizer of

$$S_t^2(\beta,\gamma) = \sum_{i=t}^{n}(Y_i - \beta_0 - \beta_1 X_i)^2$$

For $t = 1, \ldots, n-1$ we obtain a sequence of functions $S_t^2(\hat{\beta}(t),\gamma)$ which are segments of $S^2(\beta,\gamma)$ like it is given in (5).

The process of estimating the parameters in the second phase is carried out sequentially. It starts by estimating the parameters based on all observations. In this case t equals to the number of the step. Next, in each following (t-th) step the parameters are estimated using the $n-t+1$ observations and eliminating the first $t-1$ observations. This process should be continued as long as the determination coefficient R^2 increases. The step, in which the biggest value of the determination coefficient is obtained, gives estimates $\hat{\beta}_0(t)$ and $\hat{\beta}_1(t)$ of the parameters for the second phase. In consequence it may be expected that the transition point is less then X_t and its estimate is calculated using the constraint (3), i.e.

$$\hat{\gamma} = \frac{\tau - \hat{\beta}_0(t)}{\hat{\beta}_1(t)}.$$

Therefore in our procedure we determine an estimate of the unknown transition parameter γ, corresponding to the highest value of R^2 for the second phase. The proposed procedure is illustrated in Section 4.

4. Example

A case study is performed in order to illustrate the proposed technique for estimating the transition point. The data contains of 21 experimental measurement of pressure head and volumetric water content for sand 4443, (UNSODA data base, [2]). The soil properties given in UNSODA are: porosity is 0.385, bulk density is 1.63 g/cm^3 and particle density is 2.65 g/cm^3. Measurements are taken using tensiometry and gamma attenuation. Fig. 1 (a) presents data from the 21 experimental measurements for sand 4443. In this example we use the measured pressure head for the SWCC regression fit and therefore we fit the relation between volumetric water content and water pressure head h. This way we do not introduce the error due to conversion of pressure head to matric suction. The volumetric water content at saturation is given in UNSODA to be equal to 0.3.

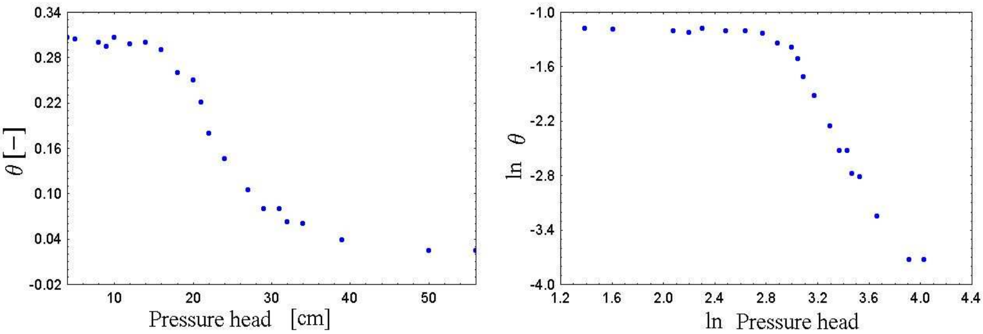

Figure 1: Sand 4443 UNSODA: (a) measured data and (b) plot after data transformation.

The following transformations $X = \ln h$, $Y = \ln \theta$ are applied to reduce the error for large pressure head values and to make the relationship linear. The plot for the transformed variables is given in Fig. 1 (b). From this plot it is seen that two intersecting straight lines represent the relationship between X and Y quite well.

First we consider a model with unknown saturated volumetric water content. The *unknown* θ_s has to be estimated through the data. Therefore we use the model

$$Y = \begin{cases} \tau, & X < \gamma \\ \beta_0 + \beta_1 X, & X \geq \gamma, \end{cases}$$

subject to $\beta_0 + \beta_1 \gamma = \tau$ with unknown parameters τ, β_0 and β_1. The estimation problem is that described in Section 3.1.

Since we have no information where approximately the transition point lies, we use a search procedure throughout the whole range of variability for independent variable. The stepwise procedure from section 3.1. is now used to obtain the optimal estimates of the parameter β_0 and β_1 and to estimate the *aev* together with θ_s. We start the search using 2 observations in the first phase and the rest 19 observations in the second phase. The results from the stepwise procedure given in Section 3.1. are summarized in Table 1. Since the R^2 is decreasing after $t = 9$ the procedure has been ceased after $t = 12$.

The optimum result is obtained for $t = 9$ with 8 observations used in the first phase and 13 observations used in the second phase. The parameters τ, β_0 and β_1 has been estimated as follows: $\hat{\tau} = -1.205$, $\hat{\beta}_0 = 5.567$, $\hat{\beta}_1 = -2.366$. The residual sum of squares, S^2, for the estimated model is 0.159 and the variance explained by the two phase linear model is R^2= 98.98%.

t	$\hat{\beta}_0(t)$	$\hat{\beta}_1(t)$	$\hat{\tau}(t)$	Final loss	R^2	$\hat{\gamma}(t)$	θ_s	aev
3	2.46	-1.46	-1.187	2.228	85.69	2.49	0.305	12.062
4	2.94	-1.61	-1.193	1.733	88.87	2.571	0.303	13.080
5	3.52	-1.78	-1.201	1.206	92.26	2.655	0.301	14.223
6	4.20	-1.98	-1.197	0.697	95.52	2.732	0.302	15.356
7	4.83	-2.16	-1.200	0.357	97.71	2.794	0.301	16.352
8	5.29	-2.29	-1.200	0.202	98.70	2.836	0.301	17.053
9	5.57	-2.37	-1.205	0.159	98.98	2.862	0.300	17.490
10	5.69	-2.40	-1.221	0.170	98.91	2.879	0.295	17.790
11	5.49	-2.35	-1.237	0.177	98.86	2.868	0.290	17.603
12	5.20	-2.27	-1.262	0.218	98.60	2.851	0.273	17.308

Table 1: Results from the stepwise estimation procedure.

The estimated value for the saturated volumetric water content is obtained using the first 8 observations and the estimated value is $\theta_s = 0.29975$ which is the same as the saturated volumetric water content given in UNSODA. Further, the transition point is estimated using the constraint (3), that gives $\hat{\gamma} = 2.86$ and consequently $a\hat{e}v = 17.49$ cm.

Now, the 95% confidence interval for γ is estimated using the equation (7). For this data $n_1 = 8$, $n_2 = 13$, $F_{1,18}^{0.05} = 4.41$ and the confidence interval is [2.79; 2.93]. Since γ is a transformed value of the aev, namely $\gamma = \ln(aev)$, the corresponding 95% confidence limits for aev are calculated using the inverse transformation. That gives the 95% confidence interval for the air entry value in cm to be [16.29; 18.79]. That is between observed values $h_8 = 16$ cm and $h_{10} = 20$ cm.

Next consideration is reasonable only if we know from other sources the saturated volumetric water content, θ_s. For instance, the UNSODA data base gives for this data $\theta_s = 0.3$.

In this case the model has the form described in Section 3.2. That is

$$Y = \begin{cases} \ln 0.3, & X < \gamma \\ \beta_0 + \beta_1 X, & X \geq \gamma, \end{cases}$$

subject to $\beta_0 + \beta_1\gamma = \ln 0.3$ with unknown parameters β_0 and β_1.

The estimation problem is that described in Section 3.2. The transition point γ should be estimated using only data from the second phase. Thus we have to decide which data are from the second, i.e. after air entry value, and use them in estimation procedure. The rest of the data will be eliminated. The stepwise procedure for this estimation is given at the end of section 3.2.

Step t	Number of observations	$\hat{\beta}_0(t)$	$\hat{\beta}_1(t)$	R^2 %
1	21	1.116	-1.052	71.893
2	20	1.690	-1.230	77.293
3	19	2.460	-1.465	84.381
4	18	2.937	-1.606	87.188
5	17	3.516	-1.777	90.545
6	16	4.204	-1.978	94.091
7	15	4.830	-2.158	96.687
8	14	5.295	-2.290	97.891
9	13	5.567	-2.366	98.101
10	12	5.687	-2.399	97.866
11	11	5.492	-2.346	97.649
12	10	5.204	-2.268	97.536
13	9	4.962	-2.202	97.027
14	8	4.601	-2.106	96.620
15	7	4.320	-2.032	96.111
16	6	4.338	-2.036	95.168

Table 2: Results from the stepwise estimation procedure.

The results from the stepwise procedure for our data are given in Table 2. The optimum result for the second phase is obtained in step 9 with 13 observations used. In this step the first 8 observations are eliminated since they are considered to be the measurements before aev. The parameter β_0 and β_1 has been estimated: $\hat{\beta}_0 = 5.567$, $\hat{\beta}_1 = -2.366$. The residual sum of squares, S^2, for the estimated model is 0.0235 and the variance explained by the model is $R^2 = 98.101\%$. The estimation of the transition point is done using the equation (3) and therefore $\hat{\gamma} = (\ln 0.3 - 5.567)/(-2.36) = 2.86$. The corresponding value of the air entry value is $a\hat{e}v = exp(\hat{\gamma}) = 17.50\,\text{cm}$.

The fit of the model to Sand 4443 UNSODA data with unknown θ_s is presented in fig.2.

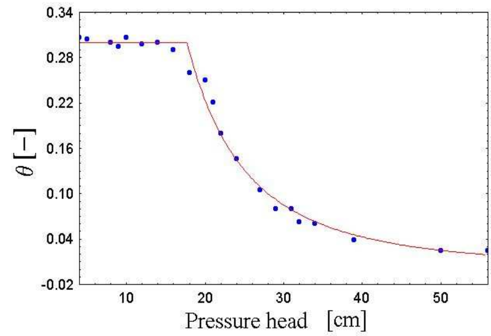

Figure 2: Sand 4443 UNSODA. Two-phase regression analysis and the fitting curve in θ versus h representation.

5. Conclusions

We presented results of the application of two-phase regression to fit SWCC data. It has been shown that if the regression of θ on ψ (or h) can be represented by two intersecting curves, one being appropriate for values below and the other for values above the *aev* then two phase regression is giving reasonable fit for the SWCC. In this case the *aev* of the SWCC is clearly a transition point. The first phase of the SWCC, in case no volume changes are present, could be taken linear with zero slope while some exponential functions are good candidates for the second phase, [15]. Several useful generalizations of the model (2) suggest themselves, for example smooth transition between two phases. Smooth transition models are discussed in [18] and [17] and could be adopted for the geotechnical data. The first phase of the multi-phase regression is not necessarily a constant. Therefore the extension of the proposed procedure is possible to cases when volume changes occur during SWCC measurements and the measured water content is not constant before the air entry value.

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