An Algorithm for Calculating the Least Limiting Water Range of Soils

Tairone Paiva Leao,* Alvaro Pires da Silva, Ed Perfect, and Cassio Antonio Tormena

ABSTRACT

The least limiting water range (LLWR) is used to estimate the optimum soil water content for plant growth based on the range of bulk density values for a given soil series under evaluation. However, the use of this methodological approach by soil scientists has been limited by the lack of a detailed description of the statistical and mathematical procedures used for its calculation. This paper describes a Statistical Analysis System (SAS) algorithm for calculation of the LLWR from bulk density, volumetric water content, water potential, and soil penetration resistance data. Since nonlinear regression techniques are used, a brief description of the theory involved in this type of statistical analysis is presented. To improve the visualization and interpretation of the LLWR results, a plotting subroutine is also described. Five soils with different textures and management conditions were used to validate the algorithm. Statistical comparison with previously published LLWR calculations showed that the new method is reliable and accurate and can substantially reduce the time and labor necessary to estimate the LLWR of soils.

The LLWR is a type of pedotransfer function used to estimate the optimum soil water content for plant growth based on quantification of the bulk density values for a given soil. However, for its computation, it is necessary to parameterize a soil water retention function $\theta(\psi)$ and a soil penetration resistance function PR(θ, D_b) (Silva et al., 1994; Leao and Silva, 2004). The LLWR is an indicator of soil physical quality that complements the available water (AW) concept. In a nondegraded and well-structured soil, the water range where plants experience adequate conditions for growth is generally defined by the field capacity in the upper end and by the wilting point in the lower end. As the soil is degraded by inadequate management practices, the bulk density tends to increase, causing a reduction of the total porosity and alterations in pore size distribution (Richard et al., 2001). This reduction in total porosity can cause aeration deficit in the rhizosphere under wet conditions. On the other hand, the increase in bulk density also translates in an increase in soil penetration resistance with drier soil conditions. The LLWR approach takes into account not only the limits of field capacity and wilting point, but also the limitations from aeration and soil penetration resistance.

The LLWR has been employed for evaluation of soil structural quality under different crops and management conditions (e.g., Zou et al., 2000; Benjamin et al., 2003; Wu et al., 2003). However, the use of the LLWR methodology among agronomists, land managers, consultants, and soil scientists has been restricted by: (i) the need for a detailed description of the nonlinear statistical parameter estimation procedures for the $\theta(\psi)$ and PR(θ, D_b) functions and (ii) the mathematical procedures for calculating the LLWR range and the critical soil bulk density (D_{bc}), where the LLWR is equal to zero.

In early work on the LLWR procedures, linear transformations of the $\theta(\psi)$ and PR(θ, D_b) functions were usually employed (Silva et al., 1994; Betz et al., 1998). This was done to avoid working with nonlinear fitting procedures. At that time, linear regression algorithms were more statistically reliable and simpler to use than most nonlinear regression software procedures. Use of nonlinear regression techniques for curve fitting has grown in the past decades (Chambers, 1973; Ratkowsky, 1990), and soil science applications are now common (Wraith and Or, 1998; Simunek and Hopmans, 2002). The reasons for the increase in use of nonlinear regression are mainly due to: (i) popularization of statistical and/or mathematical software packages containing algorithms for nonlinear regression (e.g., SAS, Origin, MathCad, and Excel); (ii) development of more robust numerical techniques for fitting nonlinear equations to data, with improved convergence properties, such as the Levenberg–Marquardt algorithm (Simunek and Hopmans, 2002); and (iii) development of methodologies for goodness of fit and residual analysis (Souza, 1998).

The objectives of this paper are to: (i) present an algorithm for estimation of the LLWR of soils using the SAS system programming language; (ii) compare this method with previously reported solutions in terms of ease of use, labor, time, and accuracy; and (iii) discuss some technical issues concerning the nonlinear curve-fitting procedures employed. The algorithm is designed in the SAS system programming language due to its widespread acceptance among the scientific community and because of its great flexibility and variety of modules and procedures.

THEORETICAL BACKGROUND

A nonlinear regression model can be written as follows (Bates and Watts, 1988; Seber and Wild, 1989):

$$y_i = f(\mathbf{x}_i; q) + \varepsilon_i (i = 1, 2, \ldots, n) \qquad [1]$$

where ε_i is a stochastic term with a mean of zero, f is the expectation function, and $\mathbf{x}_i$ is a vector of associated regressor variables or independent variables of the ith case. This model is exactly the same case as a linear regression model, except that the expected responses are nonlinear functions of a multi-

---

T.P. Leao and E. Perfect, Dep. of Earth and Planetary Sci., 306 Earth and Planetary Sci. Bldg., Univ. of Tennessee, Knoxville, TN 37996-1410; A.P. da Silva, ESALQ/USP, Av. Padua Dias, 11–Dep. Solos e Nutricao de Plantas, C.P. 9, 13418-900 Piracicaba, SP, Brazil; and C.A. Tormena, Universidade Estadual de Maringa, Centro de Ciencias Agrarias, Departamento de Agronomia, Av. Colombo, 5790–Campus Universitario, 87020900 Maringa, PR, Brazil. *Corresponding author (tleao@utk.edu).

Published in Agron. J. 97:1210–1215 (2005).
Experiment Design and Data Management
doi:10.2134/agronj2004.0229

677 S. Segoe Rd., Madison, WI 53711 USA

Abbreviations: LLWR, least limiting water range.

dimensional parameter, described here as q. That is, for nonlinear models, at least one of the derivatives of the parameters depends on at least one of the parameters (Bates and Watts, 1988).

There are a number of specialized fitting techniques for nonlinear models, and among them, the best known special class is that of nonlinear least squares models (Chambers, 1973):

$$\mathrm{F}(q) = \sum_{i=1}^{N} \quad [y_i - f_i(q)]^2 \qquad [2]$$

Good parameters values are defined as those for which the objective function $\mathrm{F}(q)$ takes on small values. The basic computational tools for nonlinear least squares are linear least squares techniques. To achieve this, all currently competitive methods begin with a linear approximation of $f_i(q)$, i.e.

$$f(q + \delta) \cong h_i + a_i\delta \qquad [3]$$

where h_i and a_i depend on the calculations performed at q and possibly at other previous points. The oldest method known is the Gauss method, which uses a simple Taylor series to approximate f_i:

$$h_i = f_i(q), \qquad a_i = \partial f_i/\partial q \qquad [4]$$

The procedure chooses δ to minimize the linear sum of squares

$$\sum_{i=1}^{N} \quad (z_i - a_i\delta)^2 \qquad [5]$$

where $z_i = y_i - h_i$.

Since the sequence of estimates produced by straightforward applications of Eq. [5] may not converge, various computation methods for nonlinear least squares have been developed (Seber and Wild, 1989). Among them, a very effective method called the Levenberg–Marquardt method has become a standard in nonlinear least squares in soil science and hydrology studies (Simunek and Hopmans, 2002). The Levenberg–Marquardt approach modifies the choice of δ in such a way as to guarantee that $\mathrm{F}(q + \delta) < \mathrm{F}(q)$; i.e., that δ is a descent step when the objective function is far from its minimum (Chambers, 1973) and switching to the inverse Hessian method as the minimum is approached (Simunek and Hopmans, 2002). Seber and Wild (1989) argue that the Levenberg–Marquardt algorithm has proved to be a good general-purpose algorithm for least squares problems, except for large residual problems where its linear convergence can be very slow or may even fail.

Quantification of the LLWR is based on fitting of a soil water retention function and a soil mechanical resistance function. The soil water retention function (SWR) in this specific case must incorporate an indicator of variability in soil structure. This structural indicator can be achieved by incorporating soil bulk density in the SWR. Silva et al. (1994) incorporated bulk density in a simple power function employed by Ross et al. (1991) for fitting water retention data

$$\theta = \alpha\psi^{\beta} \qquad [6]$$

where θ = soil volumetric water content ($\mathrm{L^3\ L^{-3}}$), ψ = water potential ($\mathrm{M\ L^{-1}\ T^{-2}}$), and α and β = fitting parameters.

Their procedure resulted in a three-parameter equation with flexible fitting properties for characterizing the influence of bulk density on soil water retention phenomena (Betz et al., 1998; Leao et al., 2004):

$$\theta = \exp(a + bD_{\mathrm{b}})\psi^{c} \qquad [7]$$

where D_{b} = soil bulk density ($\mathrm{M\ L^{-3}}$) and a, b, and c = fitting parameters.

The soil mechanical resistance function is based on the equation proposed by Busscher and Sojka (1987) (Busscher, 1990; Silva et al., 1994; Betz et al., 1998; Leao et al., 2004):

$$\mathrm{PR} = d\theta^{e}D_{\mathrm{b}}^{f} \qquad [8]$$

where PR = soil penetration resistance ($\mathrm{M\ L^{-1}\ T^{-2}}$), D_{b} = soil bulk density ($\mathrm{M\ L^{-3}}$), and d, e, and f = fitting parameters.

Equations [7] and [8] can easily be linearized by logarithmic transformation (Silva et al., 1994; Betz et al., 1998; Zou et al., 2000). However, we choose not to use this transformation because (i) given the availability of efficient nonlinear algorithms, the usefulness of linearization is somewhat diminished (Seber and Wild, 1989) and (ii) the transformation of the data usually involves a transformation of the stochastic term too, which affects the assumptions of the least squares method (Bates and Watts, 1988).

MATERIALS AND METHODS

Code Development

The computational tools employed to evaluate the LLWR are the SAS/STAT (SAS Inst., 1999a), SAS/GRAPH (SAS Inst., 2000), and SAS/OR (SAS Inst., 1999b) capabilities, all included in the SAS software package, release 9.0. The input data set necessary for LLWR calculations is comprised of the variables: soil bulk density coded Db, volumetric water content coded ThetaV, penetration resistance coded PR, and water potential coded Psi. The data set used to develop the algorithm was collected and described by Silva et al. (1994). Since there is a considerable amount of literature describing the theoretical aspects of the LLWR concept (Letey, 1985; Brady and Weil, 1999) as well as the data collection and laboratory analysis required to quantify the variables Db, ThetaV, PR, and Psi (Klute, 1986; Silva et al., 1994; Betz et al., 1998; Tormena et al., 1999), this paper is mainly focused on data analysis, and the reader is encouraged to consult references to obtain more information on these issues.

Input Data Set

An example of the input data set for the silt loam soil described by Silva et al. (1994) is provided. The input file for the SAS software is provided in the file SKP1994.dat, part of which is illustrated as follows:

```
1.35   0.4305   0.23   0.0020
1.43   0.4209   0.85   0.0050
1.51   0.3630   0.50   0.0080
1.60   0.3670   1.34   0.0100
1.54   0.3097   2.13   0.0333
1.43   0.3217   0.61   0.1
1.53   0.2516   2.27   0.5
....
1.58   0.2324   3.94   1.5
```

The first column contains the dry bulk density (Db) values in g $\mathrm{cm^{-3}}$, the second the volumetric water content (ThetaV) in $\mathrm{cm^3\ cm^{-3}}$, and the third and the fourth columns the penetration resistance (PR) and water potential (|Psi|) values, respectively, both in MPa. For the fitting procedures, it advisable that the number of pairs of points of $\theta(\psi, D_{\mathrm{b}})$ and $\mathrm{PR}(\theta, D_{\mathrm{b}})$ should be the same as used for the construction of a standard water retention curve. In most LLWR determination studies, 10 pairs of points are used. The number of replications for each point is usually three. It is not advisable to use less than five pairs of data points and less than three replications to assure the statistical quality of the parameter estimation procedure.

The values for the critical limits used in the calculation of the LLWR were taken from the literature (e.g., Silva et al., 1994). For our example, the soil particle density was assumed as 2.65 g cm^{-3} (Brady and Weil, 1999), the field capacity at $|-0.01|$ MPa, the wilting point at $|-1.5|$ MPa, the root-restricting soil penetration resistance value at 2.0 MPa, and the limiting air-filled porosity at 10%. However, the user is strongly recommended to change these critical limits according to his or her knowledge of the phenomena involved in these critical limits and experimental conditions. The critical limits for soil particle density (Dp), water potential at field capacity (PsiFC), wilting point (PsiWP), penetration resistance (PRc), and air-filled porosity (AFPc) are defined at the beginning of the program as SAS macro commands:

```
%LET  Dp = 2.65;
%LET  PsiFC = 0.01;
%LET  PRc = 2.0;
%LET  PsiWP = 1.5;
%LET  AFPc = 10;
```

Nonlinear Parameter Estimation and LLWR Calculation

Once the data are read, the next steps are to fit the penetration resistance and water retention functions described by Eq. [7] and [8]. This can be achieved using the SAS/STAT software capabilities. PROC NLIN (SAS Inst., 1999a), the procedure for nonlinear regression analysis, is used for estimating the fitting parameters *a*, *b*, *c*, *d*, *e*, and *f* from Eq. [7] and [8]. The METHOD = MARQUARDT option selects the Levenberg–Marquardt algorithm to solve the nonlinear least squares problem. The NOITPRINT chooses not to print the iterations of the optimization procedure. Initial guesses for the parameters are specified in the PARMS option and can be changed and/or restricted according to the convergence properties of the procedure. Since Eq. [7] and [8] are mathematically simple, the values of the guess estimates should not have a major influence on the convergence properties. From a practical perspective, the parameters from Eq. [7] have been observed to vary from −3 to −0.1 for *a*, from −0.1 to 1 for *b*, and from −0.1 to −0.01 for *c*; and the parameters from Eq. [8] have been observed to vary from 0.001 to 0.2 for *d*, from −4 to −1 for *e*, and from 0.2 to 8 for *f*, for estimations using bulk density in g cm^{-3}, volumetric water content in $\text{cm}^3\ \text{cm}^{-3}$, and penetration resistance and water potential in MPa units.

As a result of the PROC NLIN procedures, the output files OUT1 and OUT2 will contain the estimated parameter values to be used in the LLWR calculations. With the parameter estimates from PROC NLIN, Eq. [7] and [8] are manipulated to give the LLWR critical limits as functions of Db only:

```
data out1;
set out1;
ThetaPR = (&PRc/(a*Db**c))**(1/b);

data out2;
set out2;
ThetaFC = exp(d + e*Db)*&PsiFC**f;
ThetaWP = exp(d + e*Db)*&PsiWP**f;
ThetaAFP = (1 − Db/&Dp) − 0.1;
```

Here, ThetaPR is the variation of the soil water content at which the penetration resistance is greater than or equal to a critical value of 2 MPa with bulk density, ThetaFC is the variation of the soil water content at field capacity with bulk density, ThetaWP is the variation of the soil water content at the wilting point with bulk density, ThetaAFP is the variation of the water content when air-filled porosity equals 10% with bulk density. The ThetaAFP function is estimated from soil porosity by [(1 – Db/Dp) – 0.1], where Dp = soil particle density.

As described by Wu et al. (2003), there are four possibilities for calculating the LLWR, depending on the values of the functions ThetaPR, ThetaFC, ThetaWP, and ThetaAFC:

(a) If (ThetaAFP $\geq$ ThetaFC) and
(ThetaPR $\leq$ ThetaWP):
$$\text{LLWR} = \text{ThetaFC} - \text{ThetaWP}; \qquad [9]$$
(b) If (ThetaAFP $\geq$ ThetaFC) and
(ThetaPR $\geq$ ThetaWP):
$$\text{LLWR} = \text{ThetaFC} - \text{ThetaPR}; \qquad [10]$$
(c) If (ThetaAFP $\leq$ ThetaFC) and
(ThetaPR $\leq$ ThetaWP):
$$\text{LLWR} = \text{ThetaAFP} - \text{ThetaWP}; \qquad [11]$$
(d) If (ThetaAFP $\leq$ ThetaFC) and
(ThetaPR $\geq$ ThetaWP):
$$\text{LLWR} = \text{ThetaAFP} - \text{ThetaPR}. \qquad [12]$$

These possibilities can be easily implemented in SAS software as well as in most programming languages using conditional statements or the traditional “IF/THEN” blocks.

Critical Bulk Density Estimation

A subroutine for calculating the critical bulk density (Dbc), at which the LLWR equals zero, is presented here. In case the Dbc calculation is not necessary, the user should simply remove the Dbc subroutine from the code. The critical bulk density can be calculated by optimization procedures, using the Operational Research module of SAS software: the SAS/OR (SAS Inst., 1999b).

The nonlinear programming procedure PROC NLP (SAS Inst., 1999b) is used to find the critical bulk density value, where the LLWR equals zero. The Levenberg–Marquardt algorithm is also employed in this module, being selected in the program option TECH = LM. The equations that intercept when the LLWR equals zero are automatically selected among ThetaFC, ThetaWP, ThetaPR, and ThetaAFP equations and inserted as MODEL1 (For the LLWR lower limit) and MODEL2 (For the LLWR upper limit). The dummy variable *z* is optimized by least squares (see option: LSQ *z*) as z = MODEL1 − MODEL2, within the boundary values of $0 <$ Db < 2.0 g cm^{-3}. The result is the Db value where $z = 0$,

Table 1. Least squares fit of the soil water retention function: $\theta = \exp(a + bD_b)\psi^c$.†

Parameter	Estimate	Standard error	95% Confidence interval	
a	−0.9175	0.1471	−1.2117	−0.6234
b	−0.3027	0.0997	−0.5021	−0.1034
c	−0.0835	0.0042	−0.0918	−0.0752
$F = 5184.11$	$p < 0.0001$			

† θ = soil volumetric water content ($\text{cm}^3\ \text{cm}^{-3}$), D_b = soil bulk density (g cm^{-3}), and ψ = water potential (MPa).

Table 2. Least squares fit of the soil penetration resistance function: PR = $d\theta^{e}D_{b}^{f}$.†

Parameter	Estimate	Standard error	95% Confidence interval	
d	0.0827	0.0273	0.0281	0.1373
e	−1.6087	0.1762	−1.9611	−1.2564
f	3.0570	0.7870	1.4833	4.6308
F = 176.67	$p < 0.0001$			

† PR = soil penetration resistance (MPa), θ = soil volumetric water content (cm^3 cm^{-3}), and D_b = soil bulk density (g cm^{-3}).

also known as the critical bulk density (Dbc). The critical limits among PR, WP, FC, and AFP that intercept when LLWR equals zero are also qualitatively indicated as the "Intercept" variable in SAS output.

Plotting Procedures

A plotting subroutine is also included to aid and improve the evaluation of the LLWR. The procedure PROC GPLOT included in SAS/GRAPH (SAS Inst. 1999a) software capabilities is used to produce publication quality graphs. A SAS sample program was adapted to fill the LLWR area between the upper and lower limits (SAS Inst., 1990).

RESULTS AND DISCUSSION

Example Application

The code presented here was used for calculation of the LLWR for the SKP1994.dat data set (Silva et al., 1994). The results from nonlinear regression for Eq. [7] and [8] are presented in Tables 1 and 2. The *F* ratio and confidence intervals show that the nonlinear fitting was highly significant for the two functions evaluated (Tables 1 and 2) (Glantz and Slinker, 1990). The plot produced by the SAS code is presented in Fig. 1. A vertical line represents the critical bulk density (Dbc) calculated by the algorithm where the critical upper and lower limits of the LLWR intercept. Figure 1 is very similar to the figure presented by Silva et al. (1994) in their original development of the LLWR. The critical bulk density found by the SAS code (Dbc = 1.55 g cm^{-3}) was very close to the value found by Silva et al. (1994) (Dbc = 1.56 g cm^{-3}). The code outputs a SAS file that can be easily exported to electronic spreadsheets or used in further statistical analysis. Here the output file is named as FINAL and contains the Db, ThetaV, PR, Psi, ThetaPR, ThetaFC, ThetaWP, ThetaAFP, UL (LLWR upper limit), LL (LLWR lower limit), and LLWR values.

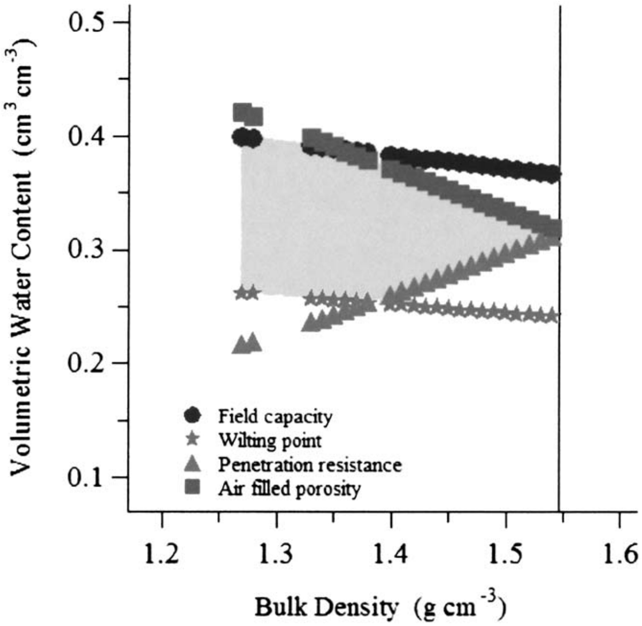

Fig. 1. Water content (θ) variation with bulk density (Db) at critical levels of field capacity (0.01 MPa), at wilting point (1.5 MPa), at air filled porosity (10%), and soil resistance (2 MPa). The vertical line represents the critical bulk density value where the least limiting water range (LLWR) equals zero. The hatched area represents the LLWR.

For an experienced researcher, it took 20 to 30 min to perform the log transformations and linear regression analyses needed for calculation of the LLWR using the standard procedure without plotting the graph. The SAS algorithm, on the other hand, takes around 1.5 s to process the same data set, including the plotting procedures.

Validation of the Algorithm

Five soils of contrasting texture and under different use and management conditions, giving a total of seven treatments, were used to validate the algorithm: silt loam Inceptisol (C1); loamy sand Alfisol (C2); sandy clay Oxisol under native vegetation (NV), continuous grazing (CG), and short-duration grazing (SG); clay Oxisol under cereal rotation (Arg); and sand Ultisol under orange orchard (Are) (Table 3). The 1:1 relationship for the LLWR estimated with the new method and the LLWR estimated by the linear method is illustrated in Fig. 2. The coefficient of the determination (r^2) varied from 0.98 to 0.99 for all soils. The hypothesis that the slope = 1 and intercept = 0 was also evaluated for

Table 3. Description of the soils used for the validation of the least limiting water range (LLWR) algorithm.

Code	Order (soil taxonomy)	Location	Use/management	Clay	Silt	Sand	Texture	Depth	Reference
				g kg^{-1}				cm	
C1	Inceptisol	Canada	Rotation corn–red clover	180	520	300	silt loam	5–10	Silva et al. (1994)
C2	Alfisol	Canada	Rotation corn–red clover	60	160	780	loamy sand	5–10	Silva et al. (1994)
NV	Oxisol	Central Brazil	Native vegetation	399	66	535	sandy clay	0–7	Leao (2002)
CG	Oxisol	Central Brazil	Continuous grazing	399	66	535	sandy clay	0–7	Leao et al. (2004)
SG	Oxisol	Central Brazil	Short-duration grazing with high stocking rates	399	66	535	sandy clay	0–7	Leao et al. (2004)
Arg	Oxisol	South Brazil	Rotation corn–wheat–soybean–oat–soybean–oat	870	92	38	clay	0–20	Tormena, unpublished data (2004)
Are	Ultisol	South Brazil	Citrus orchard	80	30	890	sand	0–15	Fidalski (2004)

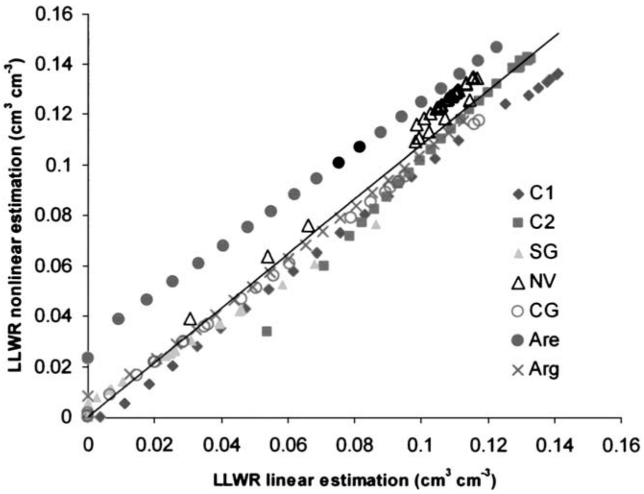

Fig. 2. A 1:1 plot of least limiting water range (LLWR) estimated using the SAS code described in this paper (nonlinear) and the LLWR estimated by conventional procedures (linear) for different soils and management. C1 = silt loam Inceptisol under corn (*Zea mays* L.)–red clover (*Trifolium pratense* L.) rotation; C2 = loamy sand Alfisol under corn and red clover rotation; NV = sandy clay Oxisol under native vegetation; CG = sandy clay Oxisol under continuous grazing; SG = sandy clay Oxisol under short-duration grazing; Arg = clay Oxisol under corn–wheat (*Triticum aestivum* L.)–soybean [*Glycine max* (L.) Merr.]–oat (*Avena sativa* L.)–soybean–oat rotation; Are = sand Ultisol under orange [*Citrus sinensis* (L.) Osbeck] orchard.

validation of the nonlinear procedure (Table 4). The intercept was statistically different from 0 in soils Are, Arg, C1, C2, and SG. The slope was statistically different from 1 in soils C2, NV, and SG.

The three cases where the slope was statistically different from 1 (C2, NV, and SG) and the sand soil (Are), where the intercept was greater than 0.02, causing a visible deviation from the 1:1 plot relationship (Fig. 2), were further investigated to determine if either the new method or the linear regression produced more reliable statistical results. Equations [7] and [8] were used to calculate θ and PR using the *a*, *b*, *c*, *d*, *e*, and *f* parameter estimates from linear and nonlinear regression. The coefficients of the lines of the PR calculated from nonlinear and linear regression parameter estimates, plotted as a function of measured PR, were compared using the *t* test from the regression ANOVA (SAS Inst., 1999a). The same procedure was used to investigate the statistical quality of the volumetric water content calculated from linear and nonlinear regression parameter estimates. The intercept was significantly different between the linear and nonlinear estimated lines for the soil C2 for PR estimation and for the soils Are, NV, and C2 for θ. However, the slope of the lines for both PR and θ was only significantly different for the sand soil (Are) (PR: $p > |t| = 0.0118$; θ: $p > |t| < 0.0001$).

The relationship of linear and nonlinear estimated θ versus observed θ and linear and nonlinear estimated PR versus observed PR was also evaluated for the sand soil (Are) using linear regression and graphs (Fig. 3 and 4). The intercept of the regression lines was only not different from zero on PR calculated from nonlinear regression ($p > |t| = 0.9917$) (Fig. 3). The coefficient of determination was the same for the lines of θ fitted by nonlinear regression versus observed θ and θ fitted by linear regression versus observed θ; $r^2 = 0.88$ (Fig. 4). For the PR lines, besides the fact that the intercept of the lines was only equal to zero for the nonlinear regression, the coefficient of determination was higher for the new method: $r^2_{\text{nonlinear}} = 0.85$ versus $r^2_{\text{linear}} = 0.79$ (Fig. 3).

Based on the coefficients of determination and the slope and intercept tests from linear regression, the overall LLWR fittings using linear and nonlinear regression

Table 4. Test for intercept = 0 and slope = 1 for the 1:1 plot of the least limiting water range (LLWR) estimated by linear versus nonlinear regression for the seven soils evaluated individually and combined ($N = 426$).

Soil	Intercept = 0	Slope = 1
	P > F	
Are	***	**0.0621**
Arg	***	**0.6363**
C1	***	**0.5534**
C2	***	***
NV	**0.6532**	***
CG	**0.2104**	**0.4928**
SG	***	***
Full data set	***	**0.1801**

***** Significant at the 0.001 probability level.**

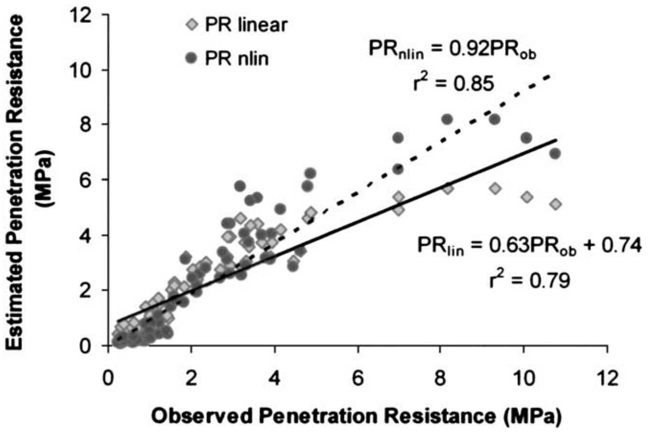

Fig. 3. Soil penetration resistance calculated using linear regression (PR_{lin}) and nonlinear regression (PR_{nlin}) coefficients plotted as a function of observed soil penetration resistance values (PR_{ob}).

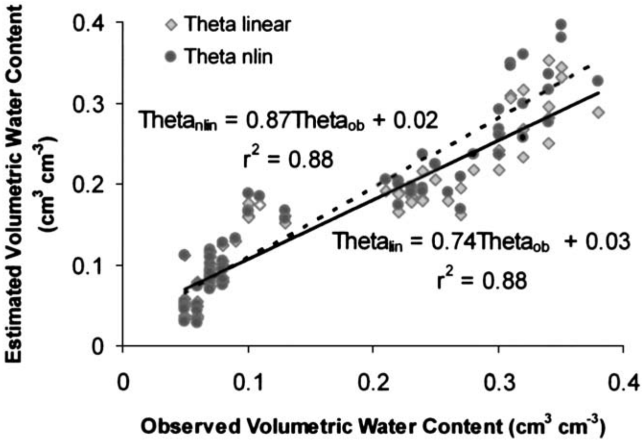

Fig. 4. Soil volumetric water content calculated using linear regression ($Theta_{lin}$) and nonlinear regression ($Theta_{nlin}$) coefficients plotted as a function of observed volumetric water content values ($Theta_{ob}$).

did not statistically differ. However, since we are basically dealing with nonlinear functions, the nonlinear fitting should be preferred, as discussed in the Theoretical Background section (also see Bates and Watts, 1988; Seber and Wild, 1989). The new procedure reduces substantially the amount of time required to perform the LLWR analysis and can be used by agronomists, land managers, consultants, and soil scientists for the evaluation of soil physical quality, without the necessity of a technical understanding of the statistical procedures involved. A general scope of the statistical analysis and computational procedures employed for quantification of the LLWR has also been presented, which should be useful in further studies on the subject.

CONCLUSIONS

The algorithm presented in this paper is a reliable and efficient statistical tool for the quantification of the LLWR of soils. It is an alternative to the time-consuming statistical analysis and plotting procedures used in the quantification and evaluation of the LLWR as an index of soil physical quality. Another advantage is that the algorithm can be modified or adapted to other software packages or programming languages according to the resources and experimental conditions of the user. The SAS code and the SKP.dat file are available electronically through contact with the first author.

ACKNOWLEDGMENTS

The authors would like to acknowledge the graduate students from the State Univ. of Maringa, Brazil: Jonez Fidalski and Marcelo Alessandro Araujo for providing the data sets for the sand and clay soils, respectively. The first author would also like to thank the anonymous reviewers for their valuable suggestions for improving the manuscript.

REFERENCES

Bates, D.M., and D.G. Watts. 1988. Nonlinear regression analysis and its applications. John Wiley & Sons, New York.

Benjamin, J.G., D.C. Nielsen, and M.F. Vigil. 2003. Quantifying effects of soil conditions on plant growth and crop production. Geoderma 116:137–148.

Betz, C.L., R.R. Allamars, S.M. Copeland, and G.W. Randall. 1998. Least limiting water range: Traffic and long-term tillage influences in a Webster soil. Soil Sci. Soc. Am. J. 62:1384–1393.

Brady, N.C., and R.R. Weil. 1999. The nature and properties of soils. 12 ed. Prentice Hall, Englewood Cliffs, NJ.

Busscher, W.J. 1990. Adjustment of flat-tipped penetrometer resistance data to a common water content. Trans. ASAE 33:519–524.

Busscher, W.J., and R.E. Sojka. 1987. Enhancement of subsoiling effect on soil strength by conservation tillage. Trans. ASAE 30:888–892.

Chambers, J.M. 1973. Fitting nonlinear models: Numerical techniques. Biometrika 60:1–13.

Fidalski, J. 2004. Soil physical properties in different management systems of the citrus interrows. (In Portuguese, with English abstract.) M.S. diss. State Univ. of Maringa, Parana, Brazil.

Glantz, S.A., and B.K. Slinker. 1990. Primer of applied regression and analysis of variance. McGraw-Hill, New York.

Klute, A. 1986. Water retention: Laboratory methods. p. 635–660. *In* A. Klute (ed.) Methods of soil analysis: Physical and mineralogical methods. 2nd ed. SSSA and ASA, Madison, WI.

Leao, T.P. 2002. Least limiting water range in different grazing systems and pasture management strategies. (In Portuguese, with English abstract.) M.S. diss. Univ. of Sao Paulo, Sao Paulo, Brazil.

Leao, T.P., and A.P. Silva. 2004. A simplified Excel algorithm for estimating the least limiting water range of soils using nonlinear regression. Sci. Agric. (Piracicaba, Braz.) 61(6):649–654.

Leao, T.P., A.P. Silva, M.C.M. Macedo, S. Imhoff, and V.P.B. Euclides. 2004. Intervalo hídrico ótimo na avaliação de sistemas de pastejo contínuo e rotacionado. Rev. Bras. Cienc. Solo 28:1–8.

Letey, J. 1985. Relationship between soil physical properties and crop production. Adv. Soil Sci. 1:277–294.

Ratkowsky, D.A. 1990. Handbook of nonlinear regression models. Marcel Dekker, New York.

Richard, G., I. Cousin, J.F. Sillon, A. Bruand, and J. Guerif. 2001. Effect of compaction on the porosity of a silty soil: Influence on unsaturated hydraulic properties. Eur. J. Soil Sci. 52:49–58.

Ross, P.J., J. Williams, and K.L. Bristow. 1991. Equations for extending water-retention curves to dryness. Soil Sci. Soc. Am. J. 55:923–927.

SAS Institute. 1990. SAS/GRAPH software: Reference. Version 6. SAS Inst., Cary NC.

SAS Institute. 1999a. SAS/STAT user's guide. Version 8. SAS Inst., Cary NC.

SAS Institute. 1999b. SAS/OR user's guide: Mathematical programming. Version 8. SAS Inst., Cary NC.

SAS Institute. 2000. SAS/GRAPH software: Reference. Version 8. SAS Inst., Cary NC.

Seber, G.A.F., and C.J. Wild. 1989. Nonlinear regression. John Wiley & Sons, New York.

Silva, A.P., B.D. Kay, and E. Perfect. 1994. Characterization of the least limiting water range of soils. Soil Sci. Soc. Am. J. 58:1775–1781.

Simunek, J., and J.W. Hopmans. 2002. Parameter optimization and nonlinear fitting. p. 139–157. *In* J.H. Dane and G.C. Topp (ed.) Methods of soil analysis: Physical methods. 3rd ed. ASA and SSSA, Madison, WI.

Souza, G.S. 1998. Introdução aos modelos de regressão linear e não-linear. Embrapa Serviço de Produção de Informação, Brasília.

Tormena, C.A., A.P. Silva, and P.L. Libardi. 1999. Soil physical quality of a Brazilian Oxisol under two tillage systems using the least limiting water range approach. Soil Tillage Res. 52:223–232.

Wraith, J.M., and D. Or. 1998. Nonlinear parameter estimation using spreadsheet software. J. Nat. Resour. Life Sci. Educ. 27:13–19.

Wu, L., G. Feng, J. Letey, L. Ferguson, J. Mitchell, B. Mccullough-Sanden, and G. Markegard. 2003. Soil management effects on the nonlimiting water range. Geoderma 114:401–414.

Zou, C., R. Sands, G. Buchan, and I. Hudson. 2000. Least limiting water range: A potential indicator of physical quality of forest soils. Aust. J. Soil Res. 38:947–958.