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ACE Guided-Transformation Method for Estimation of the Coefficient of Soil-Water Diffusivity

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Data-analytic tools for choosing transformations to increase linear association are applied to a basic problem of soil physics, the determination of the coefficient of soil-water diffusivity $D(\theta)$. Data on Manawatu sandy loam illustrate the decisions the analyst must face and the quality of the estimates that the analyst can expect.

KEY WORDS: Bulge rule; Diffusion equation; Estimation of derivatives and integrals; Transformation choice.

1. INTRODUCTION

In many problems of science and engineering, one needs to estimate derivatives and integrals of functions that are determined empirically. One problem that requires such estimates and that seems particularly interesting from a statistical perspective is the estimation of the coefficient of soil-water diffusivity $D(\theta)$. Despite being relatively unfamiliar to statisticians, this problem is a basic one of soil physics, and empirical findings are regularly reported. The feature of the problem that makes it unusual is that estimation of $D(\theta)$ typically requires determining *both* derivatives and integrals of a function that is indirectly observed.

The present approach to the estimation of $D(\theta)$ is guided by the view that statistical methods for dealing with data that exhibit strong linear associations are well developed; consequently, many nonstandard problems are best addressed by transforming the data to achieve increased linear association. The fundamental notion of straightening curves and plots is well known in the statistical literature. Still, when that simple notion is applied to a technological problem that has traditionally been addressed by ad hoc means, the outcome can be surprising. In this instance, one finds a natural estimation process that has several advantages over methods that are widely applied. The resulting approach also has the interesting feature of incorporating data-analytic exploration and conventional statistical estimations in relatively equal proportions.

In Section 2, we give a quick overview of the experiments that are typically conducted to estimate the coefficient of soil-water diffusivity. Section 3 then outlines the basic steps leading to the estimation of $D(\theta)$, and Section 4 provides the details of the approach as applied to data on Manawatu sandy loam. The analysis given there also serves to illustrate (a) the exploratory use of the alternating conditional expectation (ACE) algorithm to suggest reexpressions, (b) the application of the bulge rule to aid the search for analytically tractable reexpressions of the data, (c) the use of the $\mathbf{R}^2$ from the ACE transformed variables as a benchmark, and (d) the use of explicit analytic and numerical calculations to provide estimates of the derivative and integral expressions that determine $D(\theta)$.

Section 5 places the transformation-based approach to the estimation of $D(\theta)$ into a larger context by developing its relationship to two other problems. The first problem concerns specialized experiments for the estimation of $D(\theta)$ for θ near saturation. These experiments differ substantially from the classical horizontal infiltration experiments, and they offer an interesting direction for further statistical investigation. The second problem concerns the matching problem of reservoir engineering. It illustrates the substantial differences that can exist within the area of diffusivity estimation.

2. SOIL-WATER DIFFUSION PROBLEM

The movement of water in a horizontal column of unsaturated soil is commonly modeled by means of the one-dimensional diffusion equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left[D(\theta)\frac{\partial \theta}{\partial x}\right],$$

$$0 < x < \infty,\ 0 < t < \infty, \quad (2.1)$$

where θ is the water content of the soil, t is time, x is the position in the horizontal column, and $D(\theta)$ is the coefficient of soil-water diffusivity at the moisture level θ. Any two-variable function $\theta(x, t)$ that satisfies (2.1) can be shown (see Jost 1960, p. 31) to be a function of the single variable $\lambda = x/t^{1/2}$, which is often called the Boltzman variable. After writing $\theta(\lambda)$ for the new function of one variable, one can check that $\theta(\lambda)$ satisfies the ordinary differential equation

$$-\left[\frac{\lambda}{2}\right]\frac{d\theta}{d\lambda} = \frac{d}{d\lambda}\left[D(\theta)\frac{d\theta}{d\lambda}\right]. \quad (2.2)$$

From this equation, one can then easily obtain the expression for $D(\theta)$ that underlies our approach to its estimation:

$$D(\theta) = -\left[\frac{1}{2}\right]\frac{d\lambda}{d\theta}\int_{\theta_0}^{\theta}\lambda(u)\,du, \quad (2.3)$$

where θ_0 is the initial water content of the soil. The simultaneous appearance of both derivative and integral terms in this expression for $D(\theta)$ provides one of the most intriguing features of its estimation.

One point concerning (2.3) that probably deserves clarification is the absence of an additive term $D(\theta_0)$ on the right side. The fact that no such term is needed follows from the fact that, as $\theta \rightarrow \theta_0$, the two factors of (2.3) strike an asymptotic balance. As $\theta \rightarrow \theta_0$, one has the convergence of the integral term to 0, but the derivative term goes to ∞ in such a way that the limit of the right side of (2.3) converges to $D(\theta_0)$.

The process that has been most widely used to estimate $D(\theta)$ is the transient-flow experiment of Bruce and Klute (1956). In that experiment, water is held at a constant head and permitted to infiltrate into a horizontal column containing air-dry soil. After a fixed time interval, the column is sectioned, and the water content of the individual sections is determined either by weighing or by other methods. The data of Clothier and Scotter (1982) on Manawatu sandy loan plotted in Figure 1 are typical of those obtained through horizontal infiltration experiments. They also give an indication of some of the inherent difficulties in estimating $D(\theta)$. For instance, many smoothing methods when applied to the data of Figure 1 would lead to a virtually useless estimate of the derivative of λ with respect to θ.

In the soil-physics literature, the determination of $D(\theta)$ is sometimes described succinctly as follows: One plots θ as a function of λ and then "graphically"

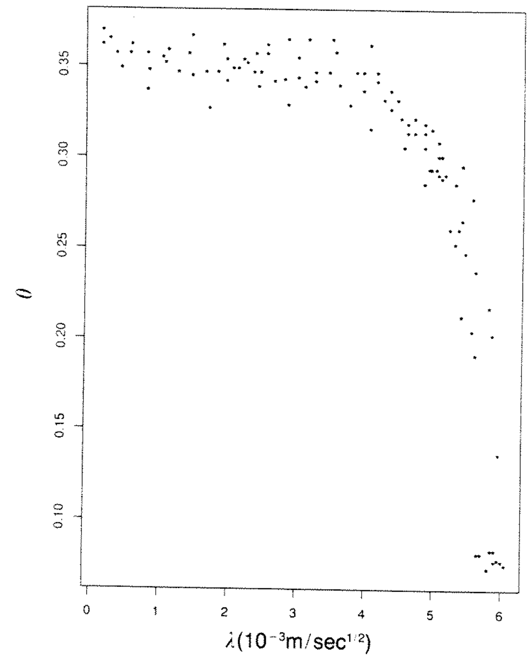

Figure 1. Scatterplot of the Volumetric Water Content, θ, Versus the Boltzman Variable λ.

determines the slope $d\lambda/d\theta$ and the area under the curve $\lambda(u)$ for $\theta_0 \le u \le \theta$. Naturally, there is a variety of ways in which the $\theta - \lambda$ plot can be used to obtain estimates of these functionals, but the procedure that is most commonly applied is probably the one given by Kirkham and Powers (1972, pp. 257–264, 266–267). A method based on splines was given by Erh (1972), and one based on piecewise parabolic fits was given by DuChateau, Nofziger, Ahuja, and Schwartzendruber (1972). Both methods provide a reasonable mechanization of the graphical determination of the terms of (2.1), but neither method has been widely applied.

In addition to these so-called "graphical determinations" of $D(\theta)$, there are approaches that rely on estimating the parameters in an assumed parametric representation for $D(\theta)$. One of the earliest such approaches is that of Gardner and Mayhugh (1958), who assumed that $D(\theta)$ can be expressed in the form

$$D(\theta) = D_d\exp(\beta\Theta), \quad (2.4)$$

where D_d is the soil-water diffusivity at air-dry content, β is a parameter to be estimated, and Θ is the dimensionless normalized water content:

$$\Theta = (\theta - \theta_0)/(\theta_s - \theta_0), \quad (2.5)$$

where θ_s is the saturated soil content and θ_0 is the initial water content.

Other parametric models that have been explored include the power-function form applied by Ahuja and Schwartzendruber (1972),

$$D(\theta) = a\theta^n/(\theta_s - \theta)^m. \tag{2.6}$$

This form for $D(\theta)$ is suggested in part by the work of Philip (1960), which provided a host of functional forms for $D(\theta)$ for which (2.1) is exactly solvable. Other parametric models were investigated by Miller and Bresler (1977), Brutsaert (1979), and Clothier and White (1981). Clothier, Scotter, and Green (1983) gave a method that applies for many of the "exact" forms of $D(\theta)$ of Philip (1960). For more details on these methods, some comparison of their relative merits, and a further parametric model of interest, consult McBride and Horton (1985).

3. ESTIMATION PROCESS

The description of the horizontal infiltration experiment and formula (2.3) for $D(\theta)$ enable us to provide a top-down view of the transformation approach to the estimation of $D(\theta)$. Several features distinguish the present approach to the estimation of $D(\theta)$ from previous methods, but the most salient is surely the explicit role given to exploratory data analysis for selecting appropriate linearizing transformations. The subsequent determination of the derivative of $\lambda(\theta)$ can then be calculated analytically, and the integral of $\lambda(\theta)$ can be calculated by either analytical or numerical means.

The details of the method we propose are possibly best explained in the context of an example such as the analysis of $D(\theta)$ of Manawatu sandy loam that is given in Section 4. Moreover, one almost has to have an honest example to detail the role of the two tools we have used to assist our transformation choice, the bulge rule and the ACE algorithm. With that said, it seems useful to have a top-down view of the proposed method. The five basic steps are the following:

Step 1. Find transformations $F(\theta)$ and $G(\lambda)$ such that the transformed data values $(F(\theta_i), G(\lambda_i))$, $1 \le i \le n$, exhibit a strong linear association. This step will be achieved by means of the ACE algorithm and the bulge rule for selecting power transformations.

Step 2. Use simple linear regression (or a more sophisticated technique like iteratively reweighted least squares) to determine values a and b, which provide an approximate functional relationship in θ and λ of the form

$$F(\theta) = a + bG(\lambda). \tag{3.1}$$

Step 3. Use a chain rule calculation to extract from (3.1) an expression for $d\lambda/d\theta$ in terms of θ.

Step 4. Use either analytic or numerical integration to determine the value of the definite integrals

$$I(\theta) = \int_{\theta_0}^{\theta} \lambda(u)\, du, \tag{3.2}$$

for all $\theta_0 \le \theta \le \theta_s$.

Step 5. Let $D(\theta)$ be estimated by the expression

$$D(\theta) = -\left[\frac{1}{2}\right] \frac{d\lambda}{d\theta} \int_{\theta_0}^{\theta} \lambda(u)\, du, \tag{3.3}$$

where the indicated derivative and integral are those determined by the results of Steps 3 and 4.

These steps are all decently explicit, except perhaps for the first. That step does require some judgment, but, as the example of Section 4 illustrates, there are useful tools to aid that judgment. Note also that Step 2 takes advantage of the fact that λ is known with negligible error, so we can more explicitly say that a and b are estimates in a model $F(\theta_i) = a + bG(\lambda_i) + \varepsilon_i$, where the error terms are independent normals with mean 0 and variance σ^2.

4. MANAWATU SANDY LOAM: EXPLORATION AND TRANSFORMATION

To understand the extent of the linear association between λ and θ that can be achieved by marginal transformations, we will call on the ACE algorithm of Breiman and Friedman (1985). This algorithm finds transformations f and g such that the empirical correlation of the transformed data $(g(\lambda_i), f(\theta_i))$, $1 \le i \le n$, is approximately maximized. If (X, Y) is a pair of jointly distributed random variables, one can define f and g as the limits of the functions f_n and g_n determined by taking $f_0(x) = x$ and $g_0(y) = y$ and applying the recursions $f_{n+1}(X) = E(g_n(Y) \mid X)$ and $g_{n+1}(Y) = E(f_n(X) \mid Y)$. The f and g determined by this process can be shown to maximize $\mathrm{corr}(f(X), g(Y))$. Naturally, if the joint distribution of X and Y is not known, one cannot find f and g precisely by this method, but one can derive an empirically based algorithm as a natural modification of the theoretical algorithm. All of our ACE computations were performed using the implementation of the empirical ACE algorithm of L. Breiman that was incorporated by Schilling (1985).

Even for the best choices of f and g, the linear association between λ and θ is imperfect. Still, the ACE-transformed variables plotted in Figure 2 exhibit substantially greater linear association than the plot of the untransformed variables given in Figure 1. Moreover, when we measure the linear association of the transformed variables in terms of $\mathbf{R}^2$, we find a respectable value of $\mathbf{R}^2 = .93$. This value provides us with a benchmark; in fact, one of the principal benefits of the ACE algorithm is that it provides a

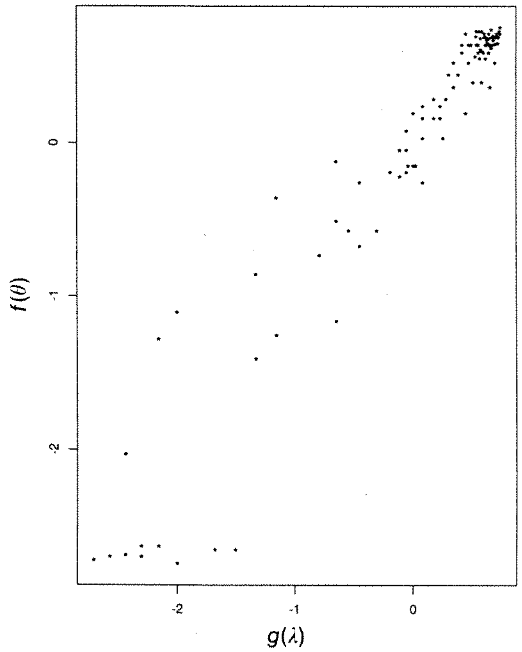

Figure 2. Scatterplot of the ACE-Transformed θ_i Versus the ACE-Transformed λ_i. This plot is used to assess linearity of the ACE transformation.

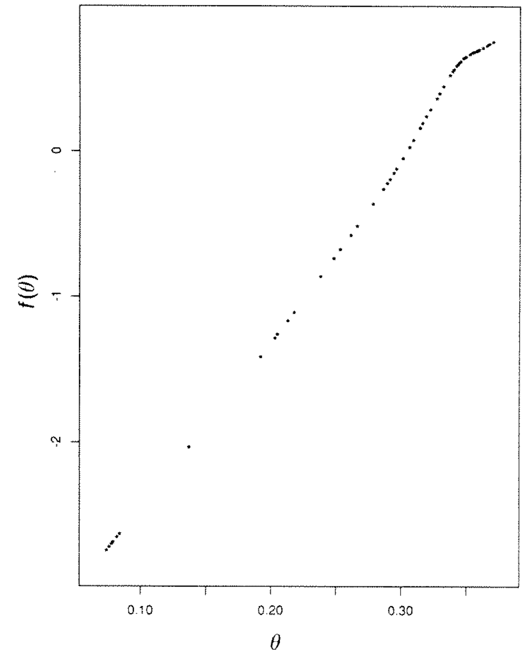

Figure 4. Scatterplot of the ACE-Transformed θ_i Versus θ_i That Is Used to Suggest a Power Transformation Approximating $f(\theta)$. Notice that the bulge rule may not be directly applicable here.

theoretical standard against which more analytically appealing transformations can be judged.

To aid in the search for such surrogates for f and g, the ACE-transformed variables are plotted against the untransformed variables to see if simpler functional forms might suffice. Figures 3 and 4 show the plots of $(\lambda_i, g(\lambda_i))$, $1 \le i \le n$, and $(\theta_i, f(\theta_i))$, $1 \le i \le n$, respectively.

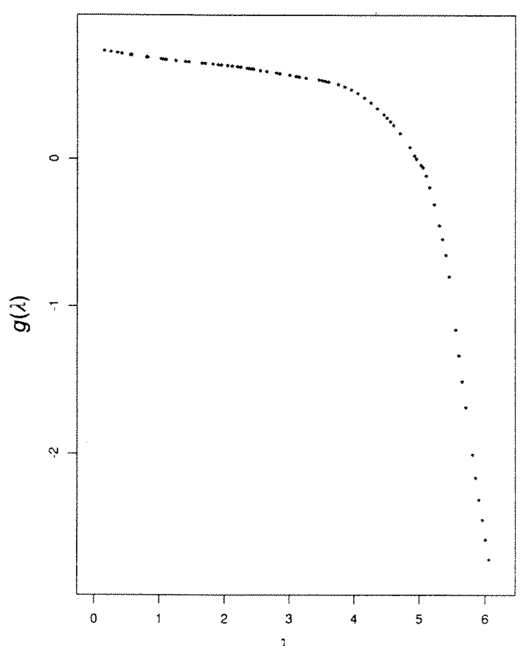

Figure 3. Scatterplot of the ACE-Transformed λ_i Versus λ_i That Is Used to Suggest a Power Transformation Approximating $g(\lambda)$.

The hunt for analytically tractable replacements for f and g is further guided by the so-called bulge rule of Mosteller and Tukey (1977). Loosely speaking, the bulge rule suggests finding an outward normal to a smoothed plot of the data and using the signs of the normal components to guide one's choice of transformation. For example, Figure 3 exhibits a bulge where both the x and y components of the outward normal are positive. The bulge rule then suggests that the variable plotted on the horizontal axis should be transformed by moving up the scale of powers. In fact, the successive examination of plots of $(\lambda_i^\alpha, g(\lambda_i))$, $1 \le i \le n$, for larger values of α continues to suggest moving up the scale of powers, and we are thus led to consider the exponential transformation. An alternative approach to this exploratory search for an appropriate transformation would be to use the method of Box and Cox (1964). The results obtained by the Box–Cox method are comparable to those obtained via the bulge rule.

When we begin a similar examination of the plot of $(\theta_i, f(\theta_i))$, $1 \le i \le n$, given in Figure 4, the bulge rule for reexpression fails to offer unambiguous advice. There may be a modest indication that we might wish to send θ down the scale of powers, but the indication is not supported when tried. Fortunately, we have recourse to a second approach that does suggest an appropriate transformation, and we can

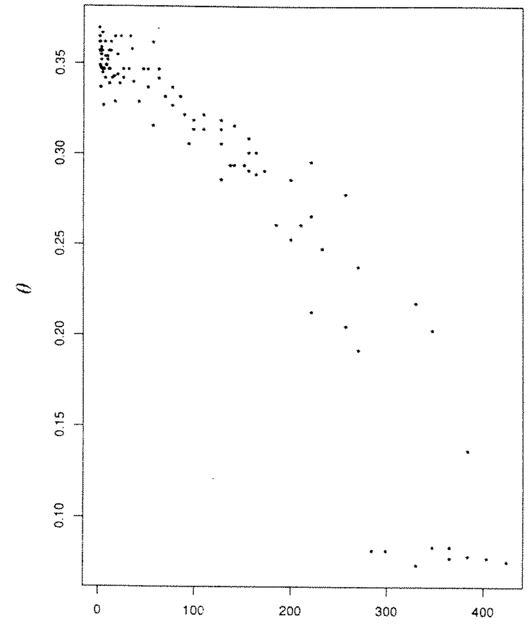

Figure 5. Scatterplot of θ_i Versus e^{λ_i}. The bulge rule suggests going up the ladder for either θ or λ.

consider the plot of θ_i versus e^{λ_i}, which is shown in Figure 5. After all, since we have settled on e^{λ} as the surrogate for $f(\lambda)$, the principal remaining task is to determine a surrogate F for f such that the scatterplot $(F(\theta_i), e^{\lambda_i})$ is approximately linearized.

The bulge rule applied to Figure 5 initially suggests that we consider a transformation F that moves θ up the ladder of powers, and successive applications of the bulge rule eventually lead us to the choice of $F(\theta) = \theta^3$. Strikingly, this transformation achieves an $\mathbf{R}^2$ of .93 that meets the level of the optimal $\mathbf{R}^2 = .93$ achieved by the ACE transformations. Moreover, when we consider the plot of θ_i^3 versus e^{λ_i} given in Figure 6, the visual impact of the linear association exhibited by this figure seems to compare well with that exhibited by the ACE-transformed variables of Figure 2. On the basis of both the quantitative evidence provided by comparing $\mathbf{R}^2$'s and the subjective evidence provided by comparison of the scatterplots of Figures 2 and 6, it seems appropriate to settle on the transformation choices of Figure 6.

5. MANAWATU SANDY LOAM: ANALYTICAL STEPS

For the Manawatu-sandy-loam data, our exploratory analysis has led us to an approximate relationship of the form

$$F(\theta) = a + bG(\lambda), \tag{5.1}$$

where $F(\theta) = \theta^3$ and $G(\lambda) = e^{\lambda}$. The coefficients in (5.1) can now be estimated by ordinary least squares, from which we obtain $a = 4.48 \times 10^{-2}$ and $b = -1.20 \times 10^{-4}$ with nominal standard errors of 5.30×10^{-4} and 3.30×10^{-6}, respectively. In Figure 7 we show a plot of the predicted values $\hat{\theta}_i^3$ versus the residuals that are obtained from fitting the model (5.1) by ordinary least squares. The residuals appear approximately homoscedastic, and we have no rea-

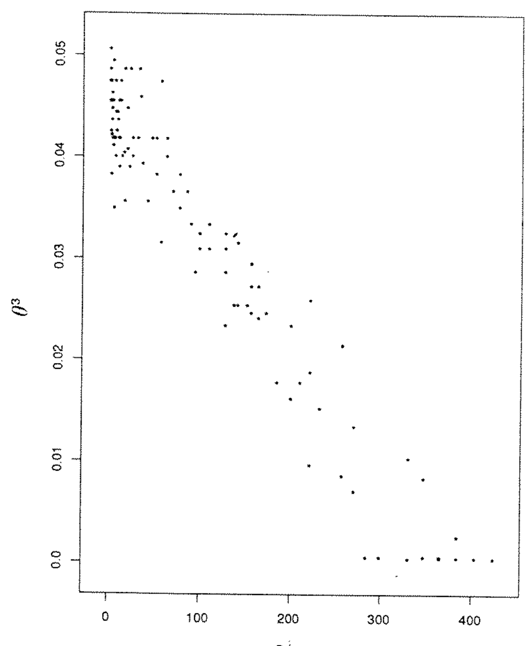

Figure 6. Scatterplot of θ_i^3 Versus e^{λ_i}. Approximate linearity is achieved with this transformation, which should be compared with the ACE transformations of Figure 2.

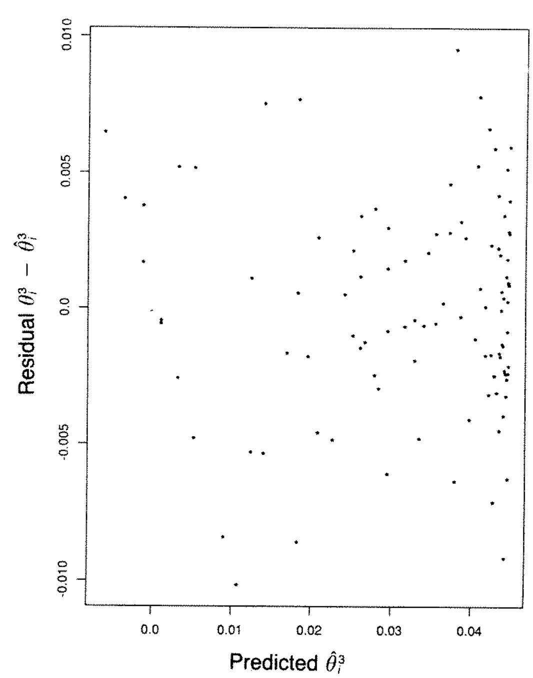

Figure 7. Scatterplot of Residuals Versus Predicted Values for the Model $\hat{\theta}_i^3 = a + be^{\lambda_i}$. Residuals appear to be approximately homoscedastic.

son to be discontent with the estimates obtained by ordinary least squares. If the scatterplot of Figure 7 had exhibited a greater heteroscedasticity, we would have probably elected to apply iteratively reweighted least squares or a similarly directed technique.

As a final check on the reasonability of the fitted model, one should consider the fit in terms of the untransformed variables as exhibited in Figure 8. This plot has no flagrant defects; indeed, it suggests that the procedure has been reasonable. Still, one feature of Figure 8 deserves comment. The principles of good experimental design suggest that one should take more observations in those regions of λ where θ changes more rapidly. Practitioners are aware of this fact and often take thinner soil sections near the wet front, although no systematic analysis of the experimental design has yet been provided.

By differentiating (5.1), we find the general relationship

$$\frac{d\lambda}{d\theta} = \frac{F'(\theta)}{bG'(\lambda)} = \frac{b^{-1}F'(\theta)}{G'(G^{-1}((F(\theta) - a)/b))}, \quad (5.2)$$

and, for the choices that were made by means of the exploratory analysis of the Manawatu-sandy-loam data, one finds a particularly simple net result:

$$\frac{d\lambda}{d\theta} = 3\theta^2(\theta^3 - a)^{-1}. \quad (5.3)$$

To obtain $D(\theta)$, it remains only to determine the integral of $\lambda(\theta) = G^{-1}((F(\theta) - a)/b)$. For the Manawatu-sandy-loam data, we find $\lambda(\theta) = \log((\theta^3 - a)/b)$, and the integral of $\lambda(\theta)$ can be determined analytically.

We are now in the position to provide the estimates for $D(\theta)$. These are given first in Figure 9 on a raw scale and again in the more appropriate log scale in Figure 10. The 99% confidence intervals given in Figure 10 probably deserve some comment. By the

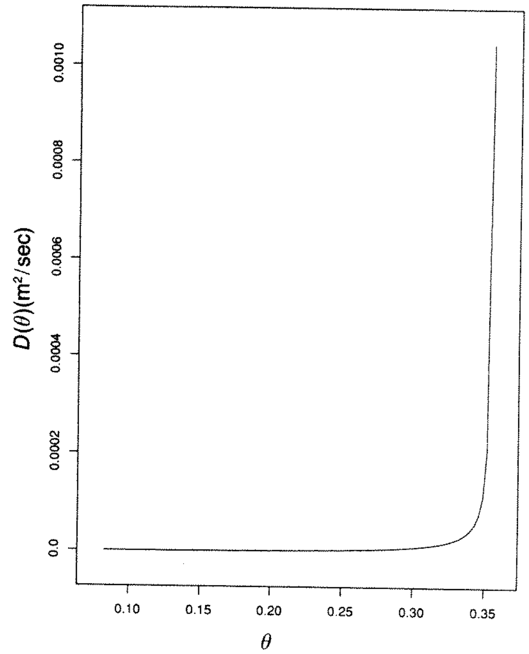

Figure 9. Plot of Soil-Water Diffusivity $D(\theta)$ Versus Moisture Content θ.

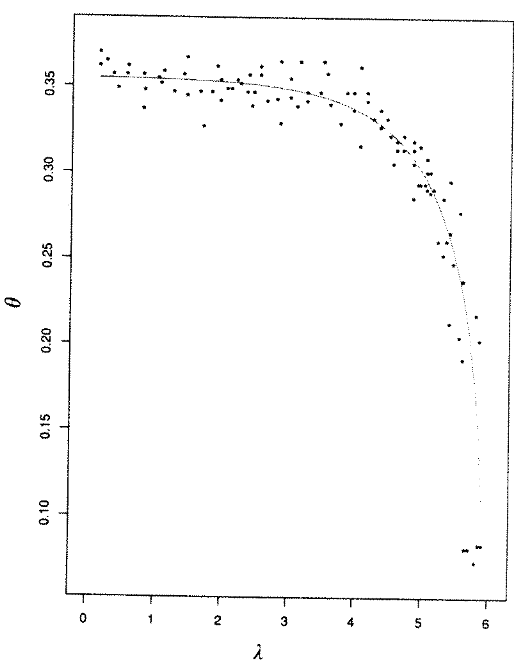

Figure 8. Scatterplot of θ_i Versus λ_i. Predicted values from the equation $\hat{\theta}_i = (a + be^{\lambda_i})^{1/3}$ are shown by the line.

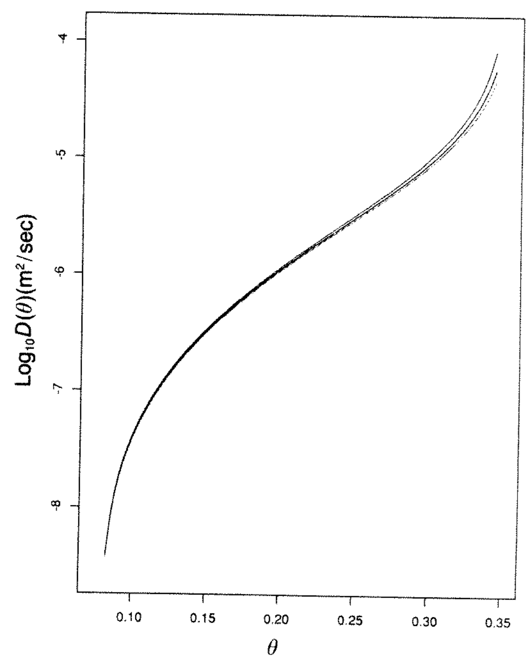

Figure 10. Plot of Log_{10} of Soil-Water Diffusivity Versus θ and the Associated 99% Upper and Lower Confidence Intervals.

usual least squares theory, one can obtain the joint distribution of the estimates $\hat{a}$ and $\hat{b}$ of the parameters of Equation (5.1). We then calculated 10^4 pseudorandom observations (a_i, b_i) with the same joint distribution as $(\hat{a}, \hat{b})$. For each θ in a set of 100 evenly spaced values, we then calculated $D_i(\theta)$ based on (a_i, b_i). Finally, we set $D^*(\theta)$ and $D_*(\theta)$ equal to the upper and lower 1% points of $\{D_i(\theta): 1 \le i \le 10^4\}$, and used these values to provide our estimates of the upper and lower values of the confidence bounds in Figure 10. The extreme narrowness of these confidence bounds is fundamentally a reflection of the small standard errors of $\hat{a}$ and $\hat{b}$. One essential observation concerning these confidence bounds is that their width increases greatly as θ approaches the saturation level θ_s. This feature is endemic to the problem of estimating $D(\theta)$, and one would have been alarmed if the confidence bounds on $D(\theta)$ did not degrade as θ approached saturation.

The desire to know how well we have done is natural but frustrating. In fact, one faces today almost the same situation as when Bruce and Klute (1956) observed, "There is unfortunately no standard against which diffusivity values can be checked" (p. 462). The estimates of Figures 9 and 10 pass the tests of physical reasonability and exhibit reasonable consistency with the results obtained by other methods, such as those of McBride and Horton (1985). We are, therefore, at a point that has confronted all others who have attempted to estimate $D(\theta)$. We have an estimate that appeals to our theoretical sensitivities, but, on the basis of current experimental evidence, we cannot argue that the present estimate is indisputably better than those obtained earlier. This fact is part of the interactive process between theory and experiment, and from the beginning of this investigation no outcome could have been expected to emerge with an ironclad claim on the truth.

6. CONCLUDING OBSERVATIONS

The problem of estimating the coefficient $D(\theta)$ of soil-water diffusivity is one that deserves the attention of statisticians. The approach explored here is natural from the point of view of contemporary data analysis; yet in comparison to commonly applied analyses, the present approach offers some substantial benefits. First, the estimate for $D(\theta)$ is guaranteed to be smooth and monotone, just as one would expect from fundamental physical principles. Further, the present method permits one to be genuinely guided by the data in contrast to methods that assume parametric forms for $D(\theta)$ based on past experience or analytic convenience.

Still, it should be understood that the estimation of $D(\theta)$ is not always easy, especially for values of θ near saturation. The difficulties in that range were recognized by Bruce and Klute (1956) and were further emphasized by Morel-Seytoux and Khanji (1975). More recently, experiments to address the estimation of $D(\theta)$ near saturation were performed by Clothier and Wooding (1983) and applied by Clothier et al. (1983). These new experiments are substantially more sophisticated than the classical horizontal infiltration experiments. They rely on the use of continuous dripping of water onto a column of soil and observation of the associated periodic fluctuations in pressure potential at differing depths in a vertical soil column. These procedures appear promising, and reexamination of the associated estimations from a statistical viewpoint would be valuable.

When one looks beyond the immediate problem of estimating the coefficient of soil-water diffusivity, one finds a world of estimation problems associated with diffusion models. Some of these problems are close cognates to the problem studied here, but other problems with a strong structural resemblance are faux amis. A striking example of this phenomenon is provided by the history-matching problem of reservoir engineering that was discussed from a statistical point of view by O'Sullivan (1986).

Again, the basic problem concerns the estimation of the diffusion parameter in a model of flow through a porous medium. Specifically, one wants to estimate the coefficient $a(\mathbf{x})$ in the diffusion equation with forcing:

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} - \frac{\partial}{\partial x}\left\{a(\mathbf{x})\frac{\partial u}{\partial x}(\mathbf{x}, t)\right\} = q(\mathbf{x}, t), \quad \mathbf{x} \in \Omega,\ 0 \le t \le T. \tag{6.1}$$

Here $\mathbf{x}$ is a two-dimensional spatial variable, and one has data on scattered well pressures $u(\mathbf{x}_i, t_j)$ and forcing pressures $q(\mathbf{x}_i, b_j)$, $1 \le i \le m$, $1 \le j \le l$.

Three essential facts separate the reservoir-matching problem from the problem of estimating soil-water diffusivity. First, the spatial variable is necessarily two dimensional, so there is no possibility of a reduction to an ordinary differential equation like (2.2). Second, time plays an essential role in (6.1), whereas in the analysis of (2.1) time had only the modest role of scaling the Boltzman variable $\lambda = x/t^{1/2}$. Finally, in (6.1) one has to deal with a complex forcing term. The presence of a modest forcing term does not automatically remove one from the domain of the present analyses—for example, the methods applied here can be modified for use on vertical infiltration experiments in which one has a forcing term because of gravity. But forcing terms with the complexity of those present in the reservoir-matching problem are of a different order, and their presence takes one into a different realm.

The two problems just sketched should serve to suggest that the subject of diffusivity estimation is quite broad. In fact, our original problem of estimating soil-water diffusivity lies at the beginning of a whole scale of challenging problems that appear ripe for statistical exploration. We hope that the steps taken here provide some introduction and encouragement to statisticians who would engage the many difficult diffusivity estimation problems that remain.

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