Title

New standards for probabilistic fitting of saturated hydraulic conductivity

ISBN

9780784409275

Author

Loáiciga, HA

Publication Date

2007-12-01

Peer reviewed

New standards for probabilistic fitting of saturated hydraulic conductivity

Hugo A. Loáiciga[1], Ph.D., P.E.

Abstract

The KSTAT Standard Committee of the Environmental Water Resources Institute (EWRI) and the American Society of Civil Engineers (ASCE) initiated activities in year 2005. Over the last two years, the KSTAT Committee has produced two preliminary standard-guidance documents expected to be published by ASCE following public review. This paper summarizes the key methods presented in the two standard-guidance documents, highlighting the potential areas of application in groundwater hydrology and geotechnical engineering.

Introduction: why probabilistic modeling of saturated hydraulic conductivity

It has been long recognized that the saturated hydraulic conductivity (K_0) exhibits a variability in aquifers that can best be described probabilistically, that is, as though K_0 were truly governed by a probability density function (pdf) from which "realizations" are drawn. In the case of aquifers, the realizations are measurements of K_0 made at various locations within an aquifer using the same measurement device or method. If K_0 can be modeled with the same probability density function within an aquifer, then the aquifer is said to be statistically homogeneous. Thus, at any arbitrary location within an aquifer, K_0 follows the same univariate pdf, say lognormal, log-gamma, gamma, exponential, beta, or other. This paper is concerned with the univariate pdf of K_0, as opposed to multivariate pdfs that describe the joint occurrence of K_0 at various aquifer locations simultaneously. It turns out that most practical applications in groundwater hydrology are well-covered by using univariate pdfs and a covariance model to describe the spatial statistical interdependence of K_0. Evidently, statistical homogeneity requires that the covariance of K_0 be unique within the aquifer, as well. Field conditions that deviate from statistical homogeneity require tools of analysis that fall outside the scope of this paper.

[1] Professor, Department of Geography/UC SB Santa Barbara CA 93106; hugo@geog.ucsb.edu

KSTAT-1: standard guidance 1 on fitting K_0 with pdfs

Lognormal pdf. Two pdfs are recommended in ASCE (2007a) to model K_0. The first is the lognormal pdf, in which case the log-conductivity $Y = ln\, K_0$ is normally distributed with average μ_Y and standard deviation σ_Y. For *Y* to be normally distributed its coefficient of skew must be zero or near zero, $|C_{sY} \le 0.05|$, specifically, on account of the symmetry of the normal pdf. The normal pdf of *Y* is:

$$f_Y(y) = \frac{1}{\sigma_Y \cdot \sqrt{2\pi}} \cdot exp\left[-\frac{1}{2}\left(\frac{y-\mu_Y}{\sigma_Y} \right)^2 \right] \qquad -\infty \le y \le \infty \qquad (1)$$

while the lognormal pdf of K_0 is:

$$f_{K_0}(x) = \frac{1}{x \cdot \sigma_Y \cdot \sqrt{2\pi}} \cdot exp\left[-\frac{1}{2}\left(\frac{ln\, x-\mu_Y}{\sigma_Y} \right)^2 \right] \qquad x \ge 0 \qquad (2)$$

In equation (1) and (2) the average μ_Y and standard deviation σ_Y are replaced by their sample estimates when implementing them for the purpose of modeling K_0 probabilistically.

The p-th quantile of lognormally distributed K_0 (denoted by x_p), where 0 < *p* < 1, is defined by the following probability statement:

$$P(K \le x_p) = p \qquad 0 < p < 1 \qquad (3)$$

which represents the probability that K_0 be equal to or less than the quantile x_p. Calculate the *p*-th quantile using the following equation:

$$x_p = exp\left(\overline{Y} + z_p\, \overline{\sigma}_Y \right) \qquad (4)$$

in which z_p is the p-th quantile of a standardized normal variable (*Z*), that is, with zero mean and unit standard deviation:

$$P(Z \le z_p) = p \qquad (5)$$

Log-gamma pdf. The second pdf recommended in ASCE (2007a) is the log-gamma pdf. This pdf is recommended for use whenever K_0 is non-symmetric, that is, when the coefficient of skew of log-conductivity is neither zero nor near zero, or whenever $|C_{sY}| > 0.05$ to be specific. The log-gamma pdf of K_0 is:

$$f_{K_0}(x) = \frac{\left(\frac{ln(x)-\theta_Y}{\beta_Y} \right)^{\alpha_Y} \left| ln(x)-\theta_Y \right|^{-1} e^{-\left(\frac{ln(x)-\theta_Y}{\beta_Y} \right)}}{x\, \Gamma(\alpha_Y)} \qquad (6)$$

where *x* represents the value of K_0 at which the log-gamma pdf is calculated; α_Y, β_Y, and θ_Y are the shape, scale, and upper or lower bound parameters of the log-gamma pdf, respectively. The log-gamma pdf may have either a lower bound:

World Environmental and Water Resources Congress 2007

$$x \geq e^{\theta_Y} \quad \text{if } \beta_Y > 0 \tag{7}$$

or it may have a lower bound (equal to zero) and an upper bound simultaneously, as follows:

$$0 < x \leq e^{\theta_Y} \quad \text{if } \beta_Y < 0 \tag{8}$$

$\Gamma(\alpha_Y)$ denotes the well-known gamma function, which is defined as follows (v is a variable of integration over the range of positive real numbers):

$$\Gamma(\alpha_Y) = \int_0^{\infty} e^{-v}\, v^{\alpha_Y - 1}\, dv \tag{9}$$

The gamma function can be calculated using commercially available spreadsheets and numerical software.

Letting $\overline{Y}$, $\overline{\sigma}_Y$, and C_{sY} be the sample average, standard deviation, and coefficient of skew of log-conductivity *Y*, respectively, calculate estimates of the log-gamma parameters as follows:

$$\alpha_Y = \frac{4}{C_Y^2} \tag{10}$$

$$\beta_Y = \frac{\overline{\sigma}_Y\, C_{sY}}{2} \tag{11}$$

$$\theta_Y = \overline{Y} - \frac{2\,\overline{\sigma}_Y}{C_{sY}} \tag{12}$$

Calculate the quantiles (x_p) of K_0 as follows:

$$x_p = exp\left[\overline{Y} + \left[\frac{\psi_q C_{sY}}{2} - \frac{2}{C_{sY}}\right]\overline{\sigma}_Y\right] \tag{13}$$

in which ψ_q is defined by the following integral equations (with $0 < p < 1$):

$$\frac{1}{\Gamma(\alpha_Y)} \int_0^{\psi_q} e^{-v}\, v^{\alpha_Y - 1}\, dv = p \qquad \text{if } C_{sY} > 0 \tag{14}$$

in which $T(\alpha_Y)$ is the gamma function, and $\alpha_Y = \frac{4}{C_{sY}^2}$, or:

$$\frac{1}{\Gamma(\alpha_Y)} \int_0^{\psi_q} e^{-v}\, v^{\alpha_Y - 1}\, dv = 1 - p \qquad \text{if } C_{sY} > 0 \tag{15}$$

and $\alpha_Y = \frac{4}{C_{sY}^2}$.

Chi-squared goodness-of-fit test. The chi-squared goodness-of-fit test for K_0 is implemented as follows:

Step 1. Calculate R quantiles of K_0, denoted by $x_{\Delta p} < x_{2\Delta p} < \ldots < x_{R\Delta p}$, using equation (4) for lognormal pdf or equation (13) for log-gamma pdf. Note that in the notation $x_{r\Delta p}$, the probability corresponding to the quantile is $r \cdot \Delta p$, in which r = 1, 2, .., R, and the probability increment Δp is defined by equation (16). A suitable range for R is $4 \le R \le 9$. The quantiles $x_{r\Delta p}$, r = 1, 2, …, R, are chosen so that they define R+1 equal-probability, non-overlapping, intervals of K_0:

$$P(x_{r\Delta p} \le K \le x_{(r+1)\Delta p}) = P(K < x_{\Delta p}) = P(K > x_{R\Delta p}) = \Delta \mathrm{p} \tag{16}$$

for r = 1, 2, …, R-1, in which:

$$\Delta p = \frac{1}{R+1} \tag{17}$$

is the probability of each of the R+1 intervals of K_0 defined by the quantiles $x_{r\Delta p}$, r = 1, 2, …, R. The quantiles satisfy the probability statement:

$$P(K \le x_{r\Delta p}) = r \cdot \Delta p \qquad r = 1, 2, \ldots, R \tag{18}$$

Step 2. The expected number of K measurements that fall in any of the R+1 (equal-probability) intervals equals $n \cdot \Delta p$, in which n is the number of K measurements available. This number compares with the actual number of K measurements observed in the r-th interval, n_r, r = 1, 2, …, R+1. Calculate the test statistic:

$$D = \frac{1}{n \cdot \Delta p} \sum_{r=1}^{R+1} (n_r - n \cdot \Delta p)^2 \tag{19}$$

Step 3. Determine the chi-squared critical value associated with a 5 % significance level and $R - f$ degrees of freedom, $\chi^2_{0.05,R-f}$. The number of degrees of freedom of the chi-squared critical value is customarily R. However, f = 2 parameters ($\bar{Y}$, $\bar{\sigma}_Y$) must be estimated from K_0 data for the lognormal pdf, and f = 3 parameters (α_Y, β_Y, θ_Y) must be estimated from data for the log-gamma pdf. Therefore, the number of degrees of freedom of the chi-squared critical value becomes $R - f$.

KSAT-2: standard guidance 2 to estimate the effective K_0

Covariance and integral scales. The effective saturated hydraulic conductivity, K_e, is a statistical parameter that relates the average specific discharge to the average hydraulic gradient. ASCE (2007b) considers the case of axisymmetric K_0 and isotropic K_0. In the former case, the spatial covariance of K_0 has a unique integral scale on the plane containing the coordinal axes (x,y), denoted by the plane h, and a second integral scale along the third axis (z) perpendicular to the plane h. In the latter, isotropic, case, the covariance of K_0 has the same integral scale along the coordinal axes x, y, z. An axisymmetric exponential covariance is then written as follows:

$$C_{K_0}(r^*) = \sigma^2_{K_0} \; e^{-r^*} \tag{20}$$

where $\sigma^2_{K_0}$ denotes the variance of K_0, and the scaled separation vector *r** takes the following form:

$$r^* = \left(\left(\frac{r_h}{I_h} \right)^2 + \left(\frac{r_z}{I_z} \right)^2 \right)^{1/2} \tag{21}$$

r_h is the radial vector in the (*x*,*y*) plane (i.e., $r_h^2 = r_x^2 + r_y^2$) and r_z is the component of separation along the axis *z* perpendicular to the (*x*,*y*) plane. The integral scale I_h on the (*x*,*y*) plane is easily shown to be given by:

$$I_h = \frac{1}{\sigma^2_{K_0}} \int_0^{\infty} C_{K_0}\left(\frac{r_h}{I_h}, 0 \right) dr_h = \int_0^{\infty} e^{-\frac{r_h}{I_h}} \, dr_h \tag{22}$$

in which the second equality assumes an exponential covariance. The integral scale I_z is defined as the integral of the covariance of K_0 with respect to the coordinate *z*, while setting $r_h = 0$.

In the isotropic case, the separation vector *r** is:

$$r^* = \frac{\left(r_x^2 + r_y^2 + r_z^2 \right)^{1/2}}{I} = \frac{r}{I} \tag{23}$$

where *I* is the integral scale in all directions (isotropic porous medium). The isotropic covariance is given by equation (20), with *r** given by equation (23). The isotropic integral scale is defined by:

$$I = \frac{1}{\sigma^2_{K_0}} \int_0^{\infty} C_{K_0}(r) \, dr = \int_0^{\infty} e^{-\frac{r}{I}} \, dr \tag{24}$$

in which the second equality assumes an exponential covariance.

Results for isotropic covariance of K_0. The important case of isotropic K_0 leads to the following effective saturated hydraulic conductivity K_e:

$$3 \, K_e \int_{all\ x} \frac{f_{K_0}(x)}{x + 2K_e} dx = 1 \tag{25}$$

in which the pdf $f_{K_0(x)}$ of K_0 is any positively tested distribution whose domain is represented by "all x" values, including the lognormal and log-gamma pdfs. The integral equation (25) must be solved for K_e once the pdf has been established.

Results for axisymmetric covariance of K_0. In this case there is an effective K_0 on the plane *h* containing the axes *x, y,* K_{eh}, and a an effective K_0 along the axis *z*, K_{ez}:

World Environmental and Water Resources Congress 2007

$$2\,K_{eh}\int_{all\,x}\frac{f_{K_0}(x)}{(x-K_{eh})\eta+2K_{eh}}dx=1 \quad (26)$$

in which $f_{K_0}(x)$ is the pdf of K_0. Other terms in equation (26) are:

$$\eta=\frac{\kappa^2}{1-\kappa^2}\left[\frac{1}{\kappa\sqrt{1-\kappa^2}}\tan^{-1}\left(\sqrt{\frac{1}{\kappa^2}-1}\right)-1\right] \quad (27)$$

in which the inverse tangent function (tan^{-1}) is expressed in radians, and:

$$\kappa=\frac{I_z}{I_h}\sqrt{\frac{K_{eh}}{K_{ez}}} \quad (28)$$

I_h and I_z are the horizontal and vertical integral scales of K_0, respectively.

The vertical effective saturated hydraulic conductivity (K_{ez}) is:

$$K_{ez}\int_{all\,x}\frac{f_K(x)}{x+\eta\cdot(K_{ez}-x)}dx=1 \quad (29)$$

Equations (26) and (29) must be solved simultaneously for K_{eh} and K_{ez}.

Effective saturated hydraulic conductivity when the log-conductivity is normally distributed with very small variance. For very small variance of log-conductivity, or $\sigma_Y^2 \leq$ 0.01, calculate the effective saturated hydraulic conductivity using the sample geometric mean ($\overline{K}_G$):

$$K_e, K_{eh}, K_{ez} \cong \overline{K}_G = e^{\overline{Y}} \quad (30)$$

in which $\overline{Y}$ is the sample average of log-conductivity Y.

Acknowledgment

The contents of this paper were extracted from two draft standard-guidance documents written by the KSTAT Standards Committee of EWRI and ASCE. The standards are under review and are expected to be published by ASCE following approval. H. A. Loáiciga serves as acting chairman of the KSTAT Standard Committee. The other members of the KSTAT Standard Committee are: Nazeer Ahmed, Jerry L. Anderson, Teresa B. Culver, Macan Doroudian, Randall W. Gentry, Paul F. Hudak, Sockalingam Sam Kannappan, Conrad G. Keyes, Jr. (Vice-chairman), Miguel A. Marino, Laurent M. Meillier, Roseanna Neupauer, Willard A. Murray, George F. Pinder, Kok-Kwang Phoon, Anand J. Puppala, Donna Rizzo, Radhey S. Sharma, Zhuping Sheng, Parmeshwar L. Shrestha, Frank T-C.Tsai, Stewart W. Taylor, Gustavious Williams, William W-G. Yeh, (Secretary), Chunmiao Zheng.

References

ASCE (2007a). *Standard guideline for fitting saturated hydraulic conductivity using probability density functions*. In review, ASCE Press, New York.

ASCE (2007b). *Standard guideline for calculating the effective saturated hydraulic conductivity*. In review, ASCE Press, New York.