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CHAPTER 5

Probability Distributions in Groundwater Hydrology

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5.0 GENERAL

Groundwater hydrology is a discipline of the earth sciences concerned with the quantitative study of water flow, water storage, chemical transport, and related processes in the subsurface. Groundwater hydrologists measure properties of soils and rocks to gain an understanding of subsurface hydrologic processes and to construct predictive models of groundwater phenomena. Those properties include, but are not limited to, porosity, permeability, hydraulic conductivity, specific storage, specific yield, and dispersivity. Because of the complex nature of geologic materials, measurements of these properties exhibit variability even in strata considered to be homogeneous on account of their origin and basic features (such as mineral composition and textural properties). For example, hydraulic conductivity measurements made at different locations in an aquifer exhibit substantial variability. Figure 5-1 exemplifies this, showing a plot of 201 measurement of hydraulic conductivity made in cohesive sediments of lacustrine origin underlying Mexico City.

The measurements of hydraulic conductivity shown in Figure 5-1 vary over five orders of magnitude. Those measurements—and those of other aquifer properties—can be analyzed using the laws of probability and statistics to obtain a proper description of the property (or variable) under study that goes beyond the calculation of its average, standard deviation, or other indicators of central tendency, dispersion, and asymmetry. The fitting of an aquifer property with a proper probability density function (pdf) is a necessary step—after its measurement in the field or in the laboratory—to arrive at a complete description of its probabilistic characteristics. Analysts can then use the fitted pdf in various analyses and design modes that provide a wider range of options than those available when the property is treated deterministically (i.e., as a nonrandom entity).

The previous paragraph should not suggest that all soil and rock properties vary over a wide numerical range. The porosity of soil and rocks, for example, takes values between 0 and 1. Table 5-1 shows the range of porosity of common rocks. Therefore, in the probabilistic analysis of porosity one must employ probability density functions defined over a finite domain, or use truncated probability functions (see, e.g., Loáiciga et al. 1992).

This chapter presents (1) several pdfs commonly used in groundwater hydrology and (2) examples of how pdfs are used to interpret aquifer properties and groundwater variables in a probabilistic manner. Several of the examples rely on hydraulic conductivity data. This is because hydraulic conductivity is an aquifer property that controls the movement of groundwater and dissolved chemicals in a fundamental manner. Besides its importance in groundwater hydrology, its variability is well suited for probabilistic analysis. In addition, hydraulic conductivity has been more extensively measured in situ or in the laboratory than any other aquifer property of relevance in groundwater hydrology. For

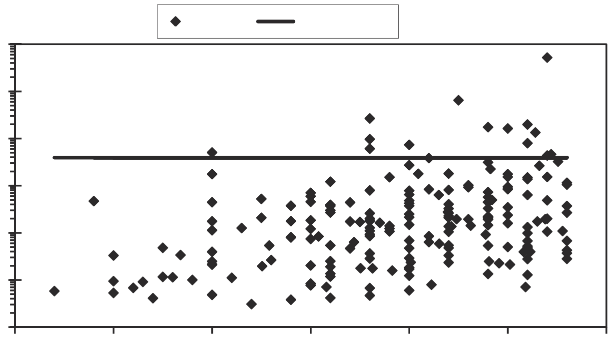

Figure 5-1. Measurement of hydraulic conductivity (K) in the lacustrine sediments underlying Mexico City. The horizontal line is the average, 3.94×10^{-8} cm/s.

Table 5-1. Range of Porosity in Near-Surface Common Rocks.

Rock type	*Range of porosity (%)*
Igneous:	
basalt	0.22–22.06
granite	1.11–3.98
Sedimentary:	
sandstone	1.62–26.40
breccia	0.78–18.73
limestone	0.27–4.36
Metamorphic:	
gneiss	0.30–2.23
marble	0.31–2.02

Source: Krynine and Judd (1957).

this reason, datasets that can be analyzed with the methods of this chapter are more common for hydraulic conductivity than for any other aquifer property. This makes the hydraulic conductivity an attractive property to work with when describing probabilistic methods amenable to the characterization of aquifer properties. This chapter uses the symbol K to represent a generic aquifer property or groundwater variable, although it is customarily used to represent the hydraulic conductivity. Some of the material presented in this chapter has been borrowed from the works of the author and collaborators (Loáiciga 2004, 2008a, 2008b, 2014; Loáiciga and Leipnik 2005; Loáiciga et al. 2006).

5.1 DEFINITIONS

5.1.1 Probability Density Function

A pdf, in the univariate case, is a mathematical formula that assigns a nonnegative value to any number contained in the domain of the pdf. They are functions of the form $f(x)$, in which x denotes any value at which the function f is calculated. The set of x values over which the function f is defined is called the domain of the pdf. The pdf integrated over its entire domain yields a value of 1. When integrated over part of its domain, it produces a probability between 0 and 1. The mathematical formula of a pdf may take many forms. Among the best known and more widely used ones are the uniform, normal (or Gaussian), the log–normal, the gamma and log–gamma, beta, exponential, Weibull, Gumbel, student *t*, and the chi-squared pdfs. In some pdfs the *x* values are strictly integer values. These pdfs are more commonly referred to as probability distributions. The binomial, Poisson, and geometric probability distributions are commonly used.

5.1.2 Correlation Coefficient

Consider two random variables X_1 and X_2 with expected values (or means) μ_1 and μ_2, and variances σ_1^2 and σ_2^2, respectively, that are correlated with correlation coefficient ρ. The following formula defines the latter:

$$\rho = \frac{E[(x_1 - \mu_1)(x_2 - \mu_2)]}{\sigma_1 \sigma_2} \tag{5-1}$$

where the symbol E denotes the expectation operator. The correlation coefficient ρ is a normalized measure of the degree of statistical association between two random variables. Its magnitude falls in the range $[-1, 1]$. A value of -1 means perfect negative correlation, a value of $+1$ denotes perfect positive correlation, and a value of zero means that the variables X_1 and X_2 are uncorrelated.

5.1.3 Spatial Correlation

Spatial correlation is a measure of the degree of statistical association among measurements of an aquifer property made at different locations in an aquifer. Positively correlated measurements occur when the spatial correlation between two measurements of the property K_1 and K_2 made at locations x_1 and x_2, respectively, ranges between 0 and 1. The closer the spatial correlation is to 1, the greater the degree of statistical association between the measurements K_1 and K_2.

5.1.4 Correlation Scale

Correlation scale is the distance between two points x_1 and x_2 beyond which the aquifer property K_1 (at x_1) and K_2 (at x_2) cease to be spatially correlated.

5.1.5 Statistical Homogeneity and Independence

Statistical homogeneity and independence of measurements are conditions that must be met when attempting to fit a pdf to a sample of measurements of an aquifer property. Statistical homogeneity implies the pdf of the property in question is the same everywhere in the aquifer or portion of aquifer in which measurements are made with a similar device or method. In this case, the measurements exhibit a constant average and a spread of values about the average devoid of spatial trends or spatial periodic patterns. Independence of measurements implies the value of the measured property at any location in an aquifer is not related in a probabilistic sense to any other of its values measured at other locations in the same aquifer. Independent measurements are uncorrelated. Property measurements can be statistically homogeneous and correlated simultaneously. In the latter instance, one must resort to geostatistics, a discipline concerned with the study of spatially correlated variables (Journel and Huijbregts 1978, Dagan 1989, Loáiciga 2010). From a physical standpoint, statistical homogeneity is approximated in the field when geological processes produce unconsolidated deposits (clays, silts, sands, gravels, or combinations of these) or consolidated deposits (also called bedrock aquifers) of similar texture, porosity characteristics, and mineral composition. Independence requires physical separations among property measurement locations that ensure the vanishing of any statistical dependence among its values. Measurement locations so chosen produce samples of measurements that are uncorrelated. The minimal spatial separation among measurements must exceed the correlation scale of the saturated hydraulic conductivity. The correlation scale can be estimated using geostatistical procedures (Loáiciga 2010).

5.2 BASIC NOTATION AND KEY STATISTICS

A sample of n measurements of an aquifer property K is assumed available for statistical inference. The individual measurements are denoted by $K_1, K_2, \ldots, K_n$, or, symbolically, by, K_j, where $j = 1, 2, \ldots, n$. The natural logarithm of K is denoted by $Y = \ln K$. The sample of Y values is denoted by Y_j ($= \ln K_j$), where $j = 1, 2, \ldots, n$. The logarithmic transformation is commonly applied to permeability, hydraulic conductivity, or other aquifer properties that are frequently found to be log–normally distributed. That is, the property is rendered normally distributed (and thus symmetric) upon undergoing the logarithmic transformation. The following subsections introduce several important statistics that describe the central tendency, the degree of spread about a measure of central tendency, and the skewness of data. The statistics are necessary in fitting pdfs to measurements of aquifer properties.

5.2.1 The Sample Average

Calculate the sample average of the property K using the following formula:

$$\overline{K} = \frac{1}{n}\sum_{j=1}^{n} K_j \tag{5-2}$$

The sample average $\overline{K}$ is an estimate of the unknown population average of K, or μ_K. The sample average is a measure of the central tendency of the data it represents.

The sample average of the log property Y is calculated with the following equation:

$$\overline{Y} = \frac{1}{n}\sum_{j=1}^{n} Y_j \tag{5-3}$$

The sample average $\overline{Y}$ is an estimate of the unknown population average of Y, or μ_Y.

5.2.2 The Geometric Mean

Calculate the sample geometric mean of K (denoted by $\overline{K}_G$) with the following equation:

$$\overline{K}_G = e^{\overline{Y}} \tag{5-4}$$

The sample geometric mean is an estimate of the (unknown) population geometric mean, $K_G = \exp(\mu_Y)$. The geometric mean is sometimes used as an effective saturated hydraulic conductivity in groundwater hydrology. The effective saturated hydraulic conductivity is a parameter that relates the average groundwater specific discharge to the average hydraulic gradient.

5.2.3 The Standard Deviation and Variance

Calculate the sample standard deviation of the property K as follows

$$\overline{\sigma}_K = \sqrt{\frac{1}{n-1}\sum_{j=1}^{n}(K_j - \overline{K})^2} \tag{5-5}$$

The sample's standard deviation $\overline{\sigma}_K$ is an estimate of the unknown population standard deviation of K, or σ_K. The sample variance of the property K is equal to $\overline{\sigma}_K^2$. The sample standard deviation measures the spread of the data about its average.

The sample standard deviation of the log property ($\overline{\sigma}_Y$) is calculated as follows:

$$\overline{\sigma}_Y = \sqrt{\frac{1}{n-1}\sum_{j=1}^{n}(Y_j - \overline{Y})^2} \tag{5-6}$$

The sample standard deviation $\overline{\sigma}_Y$ is an estimate of the unknown population standard deviation of Y, σ_Y. The sample variance of log conductivity equals $\overline{\sigma}_Y^2$.

5.2.4 The Coefficient of Skew

The sample coefficient of skew measures the degree of asymmetry of a set of measurements of the property K. It may take positive or negative values. The larger the absolute value of coefficient of skew is the more asymmetric is the pdf of the property K. A symmetric pdf, such as the normal pdf, has a coefficient of skew equal to zero. The sample coefficient of skew is calculated using the following equation:

$$C_{sK} = \frac{n}{(n-1)(n-2)}\sum_{j=1}^{n}\left(\frac{K_j - \overline{K}_j}{\overline{\sigma}_K}\right)^3 \tag{5-7}$$

The sample coefficient of skew of the log property Y is calculated as follows:

$$C_{sY} = \frac{n}{(n-1)(n-2)}\sum_{j=1}^{n}\left(\frac{Y_j - \overline{Y}_j}{\overline{\sigma}_Y}\right)^3 \tag{5-8}$$

If the log property Y is normally distributed, then its coefficient of skew equals zero. In this instance the sample coefficient of skew of the log property Y tends toward zero. In practice, if $-0.05 \le C_{sY} \le 0.05$, then the log property Y can be assumed to be normally distributed, or equivalently, that the property K follows a log–normal pdf. Otherwise, that is, if $|C_{sY}| > 0.05$, use a skewed pdf to fit the log property Y.

The average, standard deviation, and coefficient of skew can be calculated expeditiously and accurately using functions available in commercial spreadsheets and numerical software such Microsoft Excel and MATLAB.

5.3 FREQUENTLY USED PDFS IN GROUNDWATER HYDROLOGY

This chapter presents several pdfs that have been used to model aquifer properties or groundwater processes. The following sections include several applications.

5.3.1 The Log–Normal pdf

The log–normal pdf has been found to fit many types of data well, including aquifer properties such as permeability and hydraulic conductivity. Freeze (1975) provides early impetus for using the log–normal pdf as a statistical model to fit hydraulic conductivity data. Over time, the log–normal pdf has been accepted as a viable model for describing various aquifer properties (see a discussion of this topic in Loáiciga et al. 2006). Attractive features of the log–normal pdf in the modeling of some aquifer properties are (1) it can fit positively skewed data, (2) the parameters of a normally distributed log property Y [symbolically $Y \sim N(\mu_Y, \sigma_Y^2)$] are the population mean μ_Y and the population variance σ_Y^2, which are estimable using the standard sample estimators for the mean and previously introduced variance. Moreover, the quantiles of Y can be obtained straightforwardly from tabulated quantiles of the standard normal pdf $N(0, 1)$ or from statistical software. The log–normal pdf, however, cannot be used to model either skewed log data or negatively skewed aquifer data. Although the log–normal pdf allows positive lower bounds on aquifer data, it does not allow upper bounds. In contrast, the log–gamma pdf, a generalization of the gamma pdf, can fit skewed data, with upper and lower bounds, or with upper or lower bounds.

Properties of the Log–Normal pdf

Let K and θ denote an aquifer property and its lower bound, respectively, and $Y = \ln(K - \theta)$ be the log property. Evidently, $K = \exp(Y) + \theta$. The three-parameter log–normal pdf is given by the following formula (μ_Y denotes the population mean of the log property Y):

$$f_K(s) = \frac{1}{(s-\theta)\sigma_Y\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\ln(s-\theta)-\mu_Y}{\sigma_Y}\right)^2\right] \quad s > \theta \tag{5-9}$$

in which the lower bound θ is nonnegative due to physical feasibility. The lower bound θ is generally assumed equal to zero in most applications of the log–normal pdf in groundwater hydrology. The log–normal pdf in equation (5-9) implies several formulas for the property K, the log property Y, and their parameters, which follow. In these equations, for the sake of simplicity, the population means of K and Y are replaced by their sample averages $\overline{K}$ and $\overline{Y}$, respectively. The population standard deviations of K and Y are replaced by their sample estimates and $\overline{\sigma}_K$ and $\overline{\sigma}_Y$, respectively. C_{SK} denotes the population and sample coefficient of skew of the property K.

Expected Value of the Property K

$$\overline{K} = e^{\left(\overline{Y} + \frac{\overline{\sigma}_Y^2}{2}\right)} + \theta \tag{5-10}$$

The expected value is estimated by the sample average written in Equation (5-2).

Median of the Property K ($K_{0.50}$)

$$K_{0.50} = e^{\overline{Y}} + \theta \tag{5-11}$$

The geometric mean of the property K equals $K_G = \theta + \exp(\overline{Y})$, usually with $\theta = 0$, which implies the geometric mean and the median of log–normally distributed K data are equal to each other.

Equation (5-11) is convenient for estimating the lower bound θ. To do so, the sample estimator $\overline{K}_{0.50}$ is obtained and then substituted in Equation (5-11), which is then solved for an estimate of θ. Alternatively, Equation (5-10) could also be used to estimate θ. If the sample size is large (say, more than 30 values of hydraulic conductivity) and K conformed exactly to a log–normal pdf, then the estimators of θ from either equation will converge to the same value as the sample size increases. The common assumption in practical applications in groundwater hydrology is that $\theta = 0$.

Mode of the Property K

The mode (K_M) is the most likely value of K:

$$K_M = e^{\overline{Y} - \sigma_Y^2} + \theta \tag{5-12}$$

Equations (5-10), (5-11), and (5-12) show that $K_M < K_{0.50} < \overline{K}$.

Variance of the Property K **(σ_K^2)**

The following formula provides a relation between the variance of the property K and its log property Y:

$$\sigma_K^2 = e^{2\overline{Y}+\overline{\sigma}_Y^2} \cdot \left(e^{\overline{\sigma}_Y^2} - 1\right) \tag{5-13}$$

The variance of K is estimated by the square of the sample standard deviation in Equation (5-5).

Coefficient of Variation of K **(C_{vK})**

For $\theta = 0$:

$$C_{vK} = \frac{\sigma_K}{\overline{K}} = \left(e^{\overline{\sigma}_Y^2} - 1\right)^{\frac{1}{2}} \tag{5-14}$$

The coefficient of variation is a dimensionless ratio that measures the magnitude of the standard deviation of K relative to its mean. The larger the coefficient of variation is, the larger is the variability of K about its mean.

Coefficient of Skew of the Property K **(C_{sK})**

$$C_{sK} = \frac{E[K - \overline{K}]^3}{\sigma_K^3} = \frac{e^{3\,\overline{\sigma}_Y^2} - 3\,\overline{\sigma}_Y^2 + 2}{C_{vK}^3} \tag{5-15}$$

in which $\boldsymbol{C_{vk}}$ is given by Equation (5-14). The $\boldsymbol{C_{sk}}$ in Equation (5-15) is always positive. It is estimated with Equation (5-7).

Quantiles of the Property K

For $0 < p < 1$, $P(K \le K_p) = p$ defines the p-th quantile (K_p) of property K. K_p is given by

$$K_p = e^{(\overline{Y}+z_p\overline{\sigma}_Y)} + \theta \tag{5-16}$$

In Equation (5-16) z_p denotes the p-th quantile of the standard normal variate with zero mean and unit variance, which is readily obtained with ubiquitous software such as Microsoft Excel, using the function z_p = norm.s.inv(p). The quantile K_p can be obtained directly as follows:

$$K_p = e^{Y_p} + \theta \tag{5-17}$$

where the p-th quantile Y_p of the log property Y can be obtained with the norm.inv(p, $\overline{Y}$, $\overline{\sigma}_Y$) function of Microsoft Excel.

5.3.2 The Gamma pdf and Its Special Case the Exponential pdf

The gamma pdf is a versatile model that is used in many fields of science and engineering, groundwater hydrology included. Loáiciga (2004) proposes the gamma pdf as an alternative to the log–normal pdf in an analysis of stochastic groundwater flow and solute transport. Loáiciga and Leipnik (2005) apply the gamma pdf to model water-quality variables.