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Applying the Method of Lagrange Multipliers to Derive an Estimator for Unsampled Soil Properties

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ABSTRACT

Soil properties are very crucial for civil engineers to differentiate one type of soil from another and to predict its mechanical behavior. However, it is not practical to measure soil properties at all the locations at a site. In this paper, an estimator is derived to estimate the unknown values for soil properties from locations where soil samples were not collected. The estimator is obtained by combining the concept of the 'Inverse Distance Method' into the technique of 'Kriging'. The method of Lagrange Multipliers is applied in this paper. It is shown that the estimator derived in this paper is an unbiased estimator. The partiality of the estimator with respect to the true value is zero. Hence, the estimated value will be equal to the true value of the soil property. It is also shown that the variance between the estimator and the soil property is minimised. Hence, the distribution of this unbiased estimator with minimum variance spreads the least from the true value. With this characteristic of minimum variance unbiased estimator, a high accuracy estimation of soil property could be obtained.

Keywords: Lagrange Multipliers, estimator, error, variance, soil properties

INTRODUCTION

Soil properties are important for many construction purposes such as reliability and risk analysis. Identifying the properties of soil can help a civil engineer to differentiate one soil from another and to predict its mechanical behavior. For example, color, unit weight, water content and grain size distribution are some of the descriptive properties of soil that are useful for differentiating one soil from another. In addition to this, mechanical properties such as strength, deformability and permeability are useful for predicting mechanical behavior of soil [1].

Soil properties should be established at every location. However, this is not practical in reality due to cost and time constraint. It is impossible to measure soil properties at all the locations. Hence, the soil properties obtained from a site investigation are always found scattered and limited in number. Sometimes, the unknown values of soil properties at locations not included in the sampling are needed for further analysis or decision making. Hence, the estimation of the unknown values becomes essential.

In order to produce the estimation of the unknown values of the soil properties at a site, most classical statistical techniques concern only with the values of the samples collected from the site. However, geostatistics takes into account both the values and the location where the samples were collected [2]. One of the applications in geostatistics is to produce the best estimation of the unknown value at some location within a designated site. This technique is known as 'Kriging' [3]. Another estimation technique called 'Inverse Distance Method' also gives the estimation of the soil properties from locations where soil samples were not collected. In this paper, a statistical method that combines the concept of the 'Inverse Distance Method' into the technique of 'Kriging' is derived.

A Review of Kriging and Inverse Distance Method

Suppose *n* soil samples are collected from n locations at a site. The soil properties of interest are then measured from these soil samples. Suppose z_i represents the value of the soil property of interest at location x_i . Hence, $z_1, z_2, ..., z_n$ are the collected primary data on soil properties. The corresponding of the location of the soil samples are denoted by $x_1, x_2, ..., x_n$.

 x_{n} . Suppose we would like to estimate the unknown value of soil property z_0 at unsampled location x_0 , then an estimator of z_0 is needed. Suppose \hat{z}_0 represents the estimator.

A technique called 'Kriging' gives the estimation of the soil properties at unsampled locations. The term 'Kriging' is named by G. Matheron in honor of the South African mining engineer D.G. Kridge whose work on ore-grade estimation in the gold mines [4-6]. The estimation technique 'Kriging' gives the estimator, \hat{z}_0 , as follows:

$$\hat{z}_0 = \sum_{i=1}^n a_i z_i,$$
 (1)

where \hat{z}_0 = estimated value at unsampled location z_i = measured value of the soil property of interest at location a_i = Kriging weight with the constraint $\sum_{i=1}^{n} a_i = 1$.

It is noted that the estimator, \hat{z}_0 , is expressed as a linear combination of the surrounding primary data, $z_1, ..., z_n$.

Another estimation technique called 'Inverse Distance Method' also gives the estimation of the soil properties at unsampled locations. The formula used for Inverse Distance Weighting, described in Goh and Pai [7], is as below:

$$\hat{z}_0 = [z_i / (d_i + s)^p] / [1 / (d_i + s)^p],$$
(2)

- where $\hat{z}_0 =$ estimated value at unsampled location x_0 $z_i =$ measured value of the soil property of interest at location x_1
 - $d_i = \overset{x_1}{\text{distance between location of }} \hat{z}_0 \text{ and } z_i$
 - s = smoothing factor
 - p = weighting power, the most commonly used values are 1 and 2

From the formula for Inverse Distance Method, the estimated value \hat{z}_0 is inverse proportional to d_i or d_i^2 . Hence, sample points nearer to the estimated point give greater weighting than those points further away. This technique is simple and cheap to compute.

In the following section of this paper, a statistical method that combines the concept of the 'Inverse Distance Method' into the technique of 'Kriging' is derived in order to obtain another technique that consists of the advantages of the above two mentioned techniques.

DERIVATION OF A STATISTICAL METHOD TO ESTIMATE SOIL PROPERTIES

From Equation (1), it was noted that the estimator obtained from the technique of 'Kriging' is expressed as a linear combination of the surrounding primary data, $z_1, ..., z_n$ that is $\hat{z}_0 = \sum_{i=1}^n a_i z_i$. From Equation (2), the estimator in 'Inverse Distance Method' is inverse proportional to, that is the distance between location of \hat{z}_0 and z_i .

Combining the concept of the 'Inverse Distance Method' into the technique of 'Kriging', another estimator is derived, that is:

$$\hat{z}_{0}^{*} = \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} z_{i}, \qquad (3)$$

where $\hat{z}_{0}^{*} =$ estimated value at unsampled location x_{0} $z_{i} =$ measured value of the soil property of interest at location x_{i} $d_{i} =$ distance between location of \hat{z}_{0} and z_{i} $a_{i} =$ constant, subject to the constraint $\sum_{i=1}^{n} \frac{a_{i}}{d_{i}} = 1$.

Note that the constraint $\sum_{i=1}^{n} \frac{a_i}{d_i} = 1$ is to ensure that the estimator, \hat{z}_0^* , is unbiased. For an unbiased estimator, the bias is equal to zero, that is

bias =
$$E(\hat{z}_0^* - z_0) = 0$$

 $E(\sum_{i=1}^n \frac{a_i}{d_i} z_i - z_0) = 0$
 $\sum_{i=1}^n \frac{a_i}{d_i} E(z_i) - E(z_0) = 0$

It is assumed that z_0 and z_i are stationary. Thus, $E(z_i) = E(z_0) = m$ = constant, where i = 1, 2, ..., n. Hence,

$$\sum_{i=1}^{n} \frac{a_i}{d_i} m - m = 0$$
$$m \sum_{i=1}^{n} \frac{a_i}{d_i} - m = 0$$
$$m \sum_{i=1}^{n} \frac{a_i}{d_i} = m$$
$$\sum_{i=1}^{n} \frac{a_i}{d_i} = 1$$

In order to obtain the values of a_i , i = 1, 2, ..., n, the variance of error (r_0) between the estimator \hat{z}_0^* and the z_0 is minimised. The variance of error is given by:

$$Var(r_0) = Var(z_0) - 2\sum_{i=1}^n \frac{a_i}{d_i} Cov(z_0, z_i) + \sum_{i=1}^n \sum_{j=1}^n \frac{a_i a_j}{d_i d_j} Cov(z_i, z_j), \quad (4)$$

where Cov(.,.) represents the covariance function between the two variables.

The derivation of equation (4) is shown below:

$$\begin{aligned} Var(r_{0}) \\ &= Var\left(\hat{z}_{0}^{*} - z_{0}\right) \\ &= Var\left(\hat{z}_{0}^{*}\right) + Var(z_{0}) - 2Cov\left(\hat{z}_{0}^{*}, z_{0}\right) \\ &= Var\left(\sum_{i=1}^{n} \frac{a_{i}}{d_{i}} z_{i}\right) + Var(z_{0}) - 2\left[E\left(\hat{z}_{0}^{*} z_{0}\right) - E\left(\hat{z}_{0}^{*}\right)E(z_{0})\right] \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{a_{i}}{d_{i}} \frac{a_{j}}{d_{j}} Cov(z_{i}, z_{j}) + Var(z_{0}) - 2\left[E\left(\left(\sum_{i=1}^{n} \frac{a_{i}}{d_{i}} z_{i}\right)z_{0}\right) - E\left(\sum_{i=1}^{n} \frac{a_{i}}{d_{i}} z_{i}\right)E(z_{0})\right] \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{a_{i}}{d_{i}} \frac{a_{j}}{d_{j}} Cov(z_{i}, z_{j}) + Var(z_{0}) - 2\sum_{i=1}^{n} \frac{a_{i}}{d_{i}} \left[E\left(z_{i} z_{0}\right) - E\left(z_{i}\right)E(z_{0})\right] \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{a_{i}}{d_{i}} \frac{a_{j}}{d_{j}} Cov(z_{i}, z_{j}) + Var(z_{0}) - 2\sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{0}, z_{i}) \\ &= Var(z_{0}) - 2\sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{0}, z_{i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{a_{i}a_{j}}{d_{i}d_{j}} Cov(z_{i}, z_{j}) \end{aligned}$$

In order to obtain the values of $\hat{z}_0^* = \sum_{i=1}^n \frac{a_i}{d_i} z_i$, we need to solve the unknown a_i . The unknown a_i can be obtained by:

i) minimising the variance of error (r_0) ,

$$Var(r_0) = Var(z_0) - 2\sum_{i=1}^n \frac{a_i}{d_i} Cov(z_0, z_i) + \sum_{i=1}^n \sum_{j=1}^n \frac{a_i a_j}{d_i d_j} Cov(z_i, z_j),$$

ii) subject to the constraint $\sum_{i=1}^{n} \frac{a_i}{d_i} = 1$.

The method of Lagrange Multipliers is applied to solve the above mentioned optimisation problem and it is presented in the following section.

THE METHOD OF LAGRANGE MULTIPLIERS

As presented in the previous section, the unknown a_i can be obtained by

i) minimizing the variance of error (r_0) ,

$$Var(r_0) = Var(z_0) - 2\sum_{i=1}^n \frac{a_i}{d_i} Cov(z_0, z_i) + \sum_{i=1}^n \sum_{j=1}^n \frac{a_i a_j}{d_i d_j} Cov(z_i, z_j),$$

ii) subject to the constraint $\sum_{i=1}^{n} \frac{a_i}{d_i} = 1$.

The method of Lagrange Multipliers stated that, the minimum value of f, subject to the constraint g = 0, can be obtained by solving $\nabla f = \lambda \nabla g$, where λ is a Lagrange Multiplier [8]. Relating the method of Lagrange Multipliers to this case, we defined a function, $g(a_1, a_2, ..., a_n)$, where $g(a_1, a_2, ..., a_n) = \sum_{i=1}^n \frac{a_i}{d_i} - 1$. Thus, the gradient of $g(a_1, a_2, ..., a_n)$ is given by an $n \times 1$ vector

$$\nabla g = \begin{pmatrix} \frac{\partial g}{\partial a_1} \\ \frac{\partial g}{\partial a_2} \\ \vdots \\ \frac{\partial g}{\partial a_n} \end{pmatrix} = \begin{pmatrix} \frac{1}{d_1} \\ \frac{1}{d_2} \\ \vdots \\ \frac{1}{d_n} \end{pmatrix}.$$
 (5)

We defined another function $f(a_1, a_2, ..., a_n) = Var(r_0)$, that is $f(a_1, a_2, ..., a_n) = Var(z_0) - 2\sum_{i=1}^n \frac{a_i}{d_i} Cov(z_0, z_i) + \sum_{i=1}^n \sum_{j=1}^n \frac{a_i a_j}{d_i d_j} Cov(z_i, z_j)$, (6)

Thus, the gradient of $f(a_1, a_2, ..., a_n)$ is given by another $n \times 1$ vector

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial a_1} \\ \frac{\partial f}{\partial a_2} \\ \vdots \\ \frac{\partial f}{\partial a_n} \end{pmatrix} = \begin{pmatrix} -\frac{2}{d_1} Cov(z_0, z_1) + \frac{2}{d_1} \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_1) \\ -\frac{2}{d_2} Cov(z_0, z_2) + \frac{2}{d_2} \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_2) \\ \vdots \\ -\frac{2}{d_n} Cov(z_0, z_n) + \frac{2}{d_n} \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_n) \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{2}{d_{1}} \left[Cov(z_{0}, z_{1}) - \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{i}, z_{1}) \right] \\ -\frac{2}{d_{2}} \left[Cov(z_{0}, z_{2}) - \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{i}, z_{2}) \right] \\ \vdots \\ -\frac{2}{d_{n}} \left[Cov(z_{0}, z_{n}) - \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{i}, z_{n}) \right] \end{pmatrix}.$$
(7)

Hence, by using the method of Lagrange Multipliers, we obtained the minimum $f(a_1, a_2, ..., a_n) = Var(r_0)$ subject to the constraint, $g(a_1, a_2, ..., a_n) = \sum_{i=1}^n \frac{a_i}{d_i} - 1 = 0$, by solving the equation $\nabla f = \lambda \nabla g$, that is:

$$\nabla f = \lambda \nabla g$$

$$\begin{pmatrix} -\frac{2}{d_1} \left[Cov(z_0, z_1) - \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_1) \right] \\ -\frac{2}{d_2} \left[Cov(z_0, z_2) - \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_2) \right] \\ \vdots \\ -\frac{2}{d_n} \left[Cov(z_0, z_n) - \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_n) \right] \end{pmatrix} = \lambda \begin{pmatrix} \frac{1}{d_1} \\ \frac{1}{d_2} \\ \vdots \\ \frac{1}{d_n} \end{pmatrix}$$

$$\begin{pmatrix} Cov(z_0, z_n) - \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_n) \\ Cov(z_0, z_2) - \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_2) \\ \vdots \\ Cov(z_0, z_n) - \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_n) \end{pmatrix} = -\frac{\lambda}{2} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_n) - \frac{\lambda}{2} \\ \vdots \\ \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_n) - \frac{\lambda}{2} \end{pmatrix} = \begin{pmatrix} Cov(z_0, z_1) \\ Cov(z_0, z_2) - \sum_{i=1}^n \frac{a_i}{d_i} Cov(z_i, z_n) \end{pmatrix}$$

$$(8)$$

where λ is a Lagrange Multiplier.

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Including the constraint $\sum_{i=1}^{n} \frac{a_i}{d_i} = 1$ with the Equation (8) above, we obtained the following system of equations:

$$\begin{cases} \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{i}, z_{1}) - \frac{\lambda}{2} = Cov(z_{0}, z_{1}), \\ \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{i}, z_{2}) - \frac{\lambda}{2} = Cov(z_{0}, z_{2}), \\ \vdots \\ \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} Cov(z_{i}, z_{n}) - \frac{\lambda}{2} = Cov(z_{0}, z_{n}), \\ \sum_{i=1}^{n} \frac{a_{i}}{d_{i}} = 1 \end{cases}$$

$$(9)$$

The system of equations (8) can be transformed into matrix form as below:

$$\begin{pmatrix} \frac{Cov(z_{1},z_{1})}{d_{1}} & \frac{Cov(z_{2},z_{1})}{d_{2}} & \frac{Cov(z_{3},z_{1})}{d_{3}} \cdots \frac{Cov(z_{n},z_{1})}{d_{n}} & 1 \\ \frac{Cov(z_{1},z_{2})}{d_{1}} & \frac{Cov(z_{2},z_{2})}{d_{2}} & \frac{Cov(z_{3},z_{2})}{d_{3}} \cdots \frac{Cov(z_{n},z_{2})}{d_{n}} & 1 \\ \vdots & \vdots & \vdots & \vdots \\ \frac{Cov(z_{1},z_{n})}{d_{1}} & \frac{Cov(z_{2},z_{n})}{d_{2}} & \frac{Cov(z_{3},z_{n})}{d_{3}} \cdots \frac{Cov(z_{n},z_{n})}{d_{n}} & 1 \\ \frac{1}{d_{1}} & \frac{1}{d_{2}} & \frac{1}{d_{3}} & \cdots & \frac{1}{d_{n}} & 0 \end{pmatrix} \begin{pmatrix} a_{1} \\ a_{2} \\ \vdots \\ a_{n} \\ -\frac{\lambda}{2} \end{pmatrix} = \begin{pmatrix} Cov(z_{0},z_{1}) \\ Cov(z_{0},z_{2}) \\ \vdots \\ Cov(z_{0},z_{n}) \\ 1 \end{pmatrix}$$
(10)

Hence, the unknown a_i , i = 1, 2, ..., n, and the Lagrange Multiplier, λ , can be obtained by using the following formula:

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$$\begin{pmatrix} a_{1} \\ a_{2} \\ \vdots \\ a_{n} \\ -\frac{\lambda}{2} \end{pmatrix} = \begin{pmatrix} \frac{Cov(z_{1}, z_{1})}{d_{1}} & \frac{Cov(z_{2}, z_{1})}{d_{2}} & \frac{Cov(z_{3}, z_{1})}{d_{3}} \cdots \frac{Cov(z_{n}, z_{1})}{d_{n}} & 1 \\ \frac{Cov(z_{1}, z_{2})}{d_{1}} & \frac{Cov(z_{2}, z_{2})}{d_{2}} & \frac{Cov(z_{3}, z_{2})}{d_{3}} \cdots \frac{Cov(z_{n}, z_{2})}{d_{n}} & 1 \\ \vdots & \vdots & \vdots & \vdots \\ \frac{Cov(z_{1}, z_{n})}{d_{1}} & \frac{Cov(z_{2}, z_{n})}{d_{2}} & \frac{Cov(z_{3}, z_{n})}{d_{3}} \cdots \frac{Cov(z_{n}, z_{n})}{d_{n}} & 1 \\ \frac{1}{d_{1}} & \frac{1}{d_{2}} & \frac{1}{d_{3}} & \cdots & \frac{1}{d_{n}} & 0 \end{pmatrix}^{-1} \end{pmatrix}^{-1}$$

After obtaining the values of unknown a_i , i = 1, 2, ..., n, the estimated value of $\hat{z}_0^* = \sum_{i=1}^n \frac{a_i}{d_i} z_i$ can be obtained.

ADVANTAGES OF THE ESTIMATOR

The estimator that is derived in this paper has the following advantages: the estimator is unbiased and the variance of the error is minimised. The unbiased estimator enables the bias to be equal to zero, that is bias =

 $E(\hat{z}_0^* - z_0) = 0$, where z_0 is the soil property at location x_0 and \hat{z}_0^* is the estimated value derived from the estimator at location x_0 . In other words, when the bias is zero, the estimated value will be equal to the true value of the soil property. The derivation has been shown in the paper. Hence, this unbiased characteristic gives satisfactory estimation of the soil property. Figure 1 shows the difference between an unbiased estimator and a biased estimator.



Figure 1: The difference between an unbiased estimator and a biased estimator

From statistical point of view, we may find many different unbiased estimators. The distribution of each unbiased estimator is centered at the true value. However, considering the spreads of the distributions about the true value, we should choose the unbiased estimator where its distribution spreads the least from the true value. In other words, we should choose unbiased estimator with the smallest variance. In this paper, the variance between the estimator \hat{z}_0^* and the z_0 is minimised. The derivation has been shown in this paper. A smallest variance enables the distribution of the estimator closest to the true value. Figure 2 shows the difference between an unbiased estimator with minimum variance and another unbiased estimator with larger variance. The distribution of unbiased estimator of the estimator developed in this paper is very close to the true value of the soil property.



Figure 2: The difference between an unbiased estimator with minimum variance and another unbiased estimator with larger variance

The estimator derived from this paper possesses the desired characteristic of minimum variance unbiased estimator. Hence, we may obtain higher accuracy of the estimation.

CONCLUSION

In practical, soil properties are rarely measured at all the locations at a site. However, the unknown values of soil properties at unsampled locations are sometimes essential for advanced analysis. In this paper, an estimator is derived to estimate the unknown value of unsampled location. It is obtained by combining the concept of the 'Inverse Distance Method' into the technique of 'Kriging'. The derivation of the estimator involves statistical method and mathematical technique. In terms of statistical method, the concept of unbiased estimator is used, that is bias is equal to zero. With this characteristic, the estimated value from the estimator will be equal to the true value of the soil property. Another statistical method used in developing the estimator is the concept of minimum variance. Minimum variance enables the distribution of the estimator closest to the true value of the soil property. With these two constraints in developing the new estimator, a mathematical technique, the method of Lagrange Multipliers, is applied to solve this optimization problem. Hence, a minimum variance unbiased estimator is developed. Using this estimator to produce estimation for soil properties at unsampled locations, the effect of inadequate site investigation could be reduced.

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