Correlation Dimension as a Proxy for the Number of Dominant Influencing Variables for Modeling Risk of Arsenic Contamination in Groundwater

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ABSTRACT

The Correlation Dimension (CD) of an attractor provides information on the number of dominant variables present in its non-linear deterministic dynamic variability. In this study we explored the presence of a physical connection between the CD and the mathematical modeling of risk of arsenic contamination in groundwater using Logistic Regression (LR). Our database comprised a large-scale arsenic survey conducted in Bangladesh, wherein, Hossain and Sivakumar (2006) reported CD values ranging anywhere from 8 to 11. Eleven variables were considered as indicators of the aquifer's geochemical regime with potential influence on the arsenic concentration in groundwater. A total of 2048 possible combinations of influencing variables were considered as candidate LR models to delineate the impact of the number of variables on the prediction accuracy of the model. We observed that the uncertainty associated with prediction of wells as safe and unsafe by LR model declined systematically as the total number of influencing variables increased from 8 to the maximum 11. The sensitivity of the mean predictive performance also increased positively within the same range. The consistent reduction in predictive uncertainty coupled with the increased positive sensitivity of the mean predictive behavior exemplified the ability of CD to function as a proxy for the number of dominant influencing variables. Such a rapid proxy, based on non-linear dynamic concepts, appears to have considerable merit for application in current management strategies on arsenic contamination in developing countries where both time and resources are very limited.

Keywords: Nonlinear deterministic dynamics and chaos, correlation dimension, arsenic contamination, logistic regression, groundwater and Bangladesh.

INTRODUCTION

Since the large-scale discovery of arsenic contamination in the alluvial Ganges aquifers of Bangladesh, numerous studies were conducted to better understand the spatial variability of the contamination scenario (e.g., Biswas et al., 1998; Burgess et al., 2000; McArthur et al., 2001; Mukherjee and Bhattacharya, 2002; Harvey et al., 2002; van Geen et al., 2003; Yu et al., 2003; McArthur et al., 2004; Ahmed et al., 2004; Hossain et al., 2005). Most of these studies addressed the 'spatial' pattern of arsenic using geo-statistical tools and the classical notion of linear stochastic dynamics. For example, in the first country-wide study towards spatial (horizontal) characterization of the arsenic calamity, conducted by the British Geological Survey (BGS) in collaboration with the Department of Public Health and Engineering (DPHE) of Bangladesh (hereafter called 'BGS-DPHE'), an application of kriging (Journel and Huijbregts, 1978) was reported to determine the 'best' estimate of the whole nation's arsenic field at the regional scale with limited sampling information. The BGS-DPHE investigation involved the assumption that the arsenic concentration could be treated as a 'regionalized' linear stochastic random variable in space.

However, arsenic in groundwater is not a purely random occurrence. Arguing that there existed profound geological and geochemical factors controlling its variability (for example, refer to Zheng et al., 2004; McArthur et al., 2004), Hossain and Sivakumar (2005) had suggested that it was no longer defensible for the scientific community to continue to use purely geo-statistical (linear stochastic) approaches as stand-alone techniques for its spatial interpolation. Our understanding of the role played by these physical factors in arsenic contamination of groundwater continues to be enhanced by recent studies reported by, for example, Zheng et al. (2004), Akai et al. (2004) and Ahmed et al. (2004), among others. Concerns on the use of purely stochastic approaches and potential for alternative ones have been echoed by a few other studies as well (e.g. Faybishenko, 2002; Sivakumar, 2004a; Sivakumar et al., 2005). Further arguing that the current ensemble of theories in scientific literature explaining arsenic mobility (examples include: Burgess et al., 2000; McArthur et al., 2001; Harvey et al., 2002; van Geen et al., 2003) can, in principle, be mathematically represented as the cumulative effect of a finite number of dominant processes comprising three or more partial differential equations, Hossain and Sivakumar (2006) verified the existence of nonlinear deterministic and chaotic dynamic behavior in the spatial pattern of arsenic contamination in shallow wells (depth < 150 m) in Bangladesh. Using the Grassberger-Procaccia (Grassberger and Procaccia, 1983) correlation dimension algorithm, their analysis revealed Correlation Dimension (CD) values ranging anywhere from 8 to 11 depending on the region and geology. Their recent findings suggested that the arsenic contamination in space, from a chaotic dynamic perspective, was a medium- to high-dimensional problem.

Although the CD of an attractor provides information on the number of dominant variables present in its non-linear deterministic dynamic variability (Hossain and Sivakumar, 2006; Sivakumar, 2004b; Hao. 1984), current literature is not indicative of any research aimed at extracting useful information from such a chaotic paradigm that could potentially improve spatial interpolation of arsenic contamination at non-sampled locations. Hossain and Sivakumar (2005) have dwelled extensively on such possibilities for improving accuracy and cost-effectiveness of environmental management in rural and resource-limited settings of developing countries such as Bangladesh, Vietnam and India where the arsenic problem is severe. They concluded with a call for a change in the current state-of-the-art for spatial interpolation of arsenic contamination as follows: "*While there is no structural, or even philosophical, flaw in using the conventional geo-statistical approach, there is indeed ample room to argue that the geo-statistical treatment of arsenic contamination in space as a regionalized random (or stochastic) variable may constitute only an incomplete analysis of its spatial variability (even if system-dependent). Incompleteness can potentially arise from the fact that geo-statistics often fails to recognize the random looking but deterministic behavior that may be present due to self-similar (scale-invariant) factors in the continuum of the sub-surface.*"

In that spirit, this study was motivated by a need to investigate the opportunities offered by a non-linear deterministic paradigm. Specifically, we explored the presence of a physical connection between the CD and the mathematical modeling of risk of arsenic contamination in groundwater using Logistic Regression (LR). Using 11 geochemical variables that quantified the aquifer regime and hence potentially influenced the variability of arsenic concentration, we witnessed insightful evidence CD's ability to serve as a proxy for the number of dominant variables required to optimally predict contamination at non-sampled wells. To the best of our knowledge, such a preliminary insight constitutes an important finding with potentially beneficial implications on the reduction of uncertainty of risk maps produced from conventional (linear stochastic) paradigms. In the sections that follow, we provide a systematic overview of exploratory research that was carried out to understand the value of CD in modeling risk of arsenic contamination.

STUDY REGION, DATA AND CORRELATION DIMENSION ANALYSIS

We chose to study the entire region of Bangladesh as had been first surveyed by the BGS-DPHE (2001) study comprising 3534 wells. This was conducted in the manner similar to Sivakumar and Hossain (2006) for deriving the CD values. The dataset was available at http://www.bgs.ac.uk/arsenic/Bangladesh.html. Wells deeper than 150 m (and consistently below the safe limits) were excluded from the analysis, thus resulting in a set of 3085 shallow wells. For details on the study region and data, the reader is referred to the works of Hossain and Sivakumar (2006) and Hossain et al. (2005). The CD method employed by Hossain and Sivakumar (2006) used the correlation integral or function (Grassberger and Procaccia, 1983) for distinguishing between chaotic and stochastic behavior (more specifically, between low-dimensional and high-dimensional systems). While criticisms may be drawn on our use of the CD method based on limited data (i.e., a few thousand data points), a recent study by Sivakumar (2005) clearly demonstrated that the issue of large data size requirement for CD estimation is usually unfounded unless the presence of noise is widespread. Because the BGS-DPHE (2001) dataset was derived from quality-controlled measurements in the laboratory, the presence of noise in data is thus believed to be an irrelevant issue herein. The traditional application of the algorithm has been applied to data series in the continuum of time (e.g. Theiler, 1987; Sivakumar, 2005; Sivakumar et al., 2002). Hossain and Sivakumar (2006) have, however, argued that there was no compelling logic that disqualified its application to a data series in space. The CD method revealed convincing medium-to-high dimensional chaotic pattern with a country-wide dimension value ranging between 8 and 11. This subsequently led Hossain and Sivakumar (2005 and 2006) to comment subjectively that the minimum number of variables and hence the number of dominant processes required to model the spatial variability of arsenic should also range from 8-11.

LOGISTIC REGRESSION (LR)

The method of Logistic Regression (LR) has been extensively used in epidemiological studies, and more recently, has become a common technique in environmental research on modeling risk of groundwater contamination (Twarakavi and Kaluarachchi, 2005). Common regression techniques, such as the classical linear regression, relate the response variables to the influencing variables. LR relates the probability of a response variable to be greater than a threshold value to a set of influencing variables (Afifi and Clark, 1984; Helsel and Hirsch, 1992). In an LR model, regression is linear between the natural logarithm of the odds ratio for the probability of response to be less than the threshold value and influencing variables. Equation 1 mathematically summarizes the LR model used in this study as follows:

$$\ln[p/(1-p)] = \mathrm{logit}\,(p) = \alpha + \boldsymbol{\beta}\mathbf{x} \qquad (1)$$

where p is the probability of response to be greater than the safety threshold, α is a constant, $\boldsymbol{\beta}$ is a vector of slope coefficients, and $\mathbf{x}$ is a vector of influencing variables. For more details on the use of LR for modeling risk of arsenic contamination, the reader is referred to Twarakavi and Kaluarachchi (2005).

THE INFLUENCING VARIABLES

Table 1 shows the total number of 11 influencing variables defining the geochemical regime of aquifers. Most of these variables were sampled from groundwater by BGS-DPHE (2001) in Bangladesh. The minimum and maximum values of these variables (Table 1) indicate the noticeable range of variability across the whole Bangladesh. The variables chosen were: 1) depth of wells (m); 2) P (Phosphorus) (mg/l); 3) Fe (Iron) (mg/l); 4) Ba (Barium) (mg/l); 5) Mg (Magnesium) (mg/l); 6) Ca (Calcium) (mg/l); 7) SO_4 (Sulphate) (mg/l); 8) Mean Annual Precipitation (mm/day); 9) Si (Silicon) (mg/l); 10) Na (Sodium) (mg/l); 11) Mn (Manganese) (mg/l). Our choice of variables was primarily dictated by recent literature reports on the causes of arsenic mobility (such as Zheng et al., 2004; McArthur et al., 2004; Harvey et al., 2002; van Geen et al., 2003; Welch et al., 2000; among others) and the availability of accurate data. As a preliminary step, we first conducted the Spearman's Rank Correlation Coefficient test for these selected variables to verify their non-linear dependence with arsenic concentration. Because all possible combinations of influencing variables were considered during LR modeling (discussed next), results from the Spearman's test were not consequently needed for ranking of the variables according to the order of influence. The precipitation data were obtained from the Bangladesh Meteorological Department (BMD) and Bangladesh Water Development Board (BWDB). This data was derived from a network of 100 recording rainfall gauges that registered less than 5% missing data for the year 2000. The choice for precipitation as an influencing variable was governed by reports that groundwater pumping for irrigation and recharge could be one of the primary causes of arsenic mobility in the shallow geologic stratum (Harvey et al., 2002). Because recharge data were not readily available for our study, we therefore chose mean rainfall as an indicator of recharge of aquifers. For consistency, we selected precipitation data pertaining to the year 2000 when the BGS-DPHE (2001) survey was completed. The mean annual rainfall value for each well was computed by the method of Thiessen Polygons using the ArcGIS™ software (Ormsby et al., 2004).

Table 1. The selected influencing variables for Logistic Regression Modeling.

Variable	Mean	Minimum	Maximum
Well depth (m)	60.550	0.600	362.000
Ba (ppb)	87.340	2.000	1360.000
Ca (mg/L)	51.590	0.100	366.000
Fe (mg/L)	3.353	0.005	61.000
Mg (mg/L)	20.750	0.040	305.000
Mn (mg/L)	0.555	0.001	9.980
Na (mg/L)	88.936	0.700	2700.000
P (mg/L)	0.765	0.100	18.900
Si (mg/L)	20.519	0.030	45.200
SO4 (mg/L)	5.917	0.200	753.000
Precip. (cm)	86.001	25.350	596.140
As (ppb)[1]	55.205	0.500	1660.000

[1] Arsenic (As) is the dependent variable in the LR model.

METHOD OF ASSESSMENT

The dataset was divided randomly into two equal halves, with one half being employed for LR model calibration and the other half for validation. This random selection procedure was repeated 25 times within a Monte Carlo (MC) framework to assess the mean and variability of prediction of the LR model. Using one-half of each randomly selected dataset, calibration of the LR model coefficients, α and $\boldsymbol{\beta}$ was performed using ordinary least squares technique for a safety threshold of 50 ppb (Bangladesh limit). In the calibration phase, the 'p' values for Equation 1 were assigned 0-1 binary values depending on the measured concentration of arsenic (p=1; for exceeding the threshold; p=0 for being below the threshold). During the validation phase, the LR model was assessed in terms of its ability to successfully predict contamination in 0-1 binary terms according to the safety threshold at non-sampled wells (i.e., over the other half of the dataset that was not used in calibration). For this, we employed the notion of contamination risk associated with a pre-assigned probability (i.e., in this case, p=0.9). For example, if the well was predicted by the LR model as unsafe with a p value = 0.85(0.95) for a given safety threshold, then that well would be classified as uncontaminated(contaminated) according to the high risk criterion of p=0.9. The predictive power of the LR model for a given number of influencing variables was then quantified by the probability of successful classification of a well's status as contaminated or uncontaminated at untested well locations. It should be noted that the pre-assignment of a probability value to denote a risk criterion as high(low) is purely subjective and will only linearly scale up(down) the predictive behavior of LR model without altering the overall response pattern to the number of influencing variables. Hence, such our subjective assignment did not violate the overall scheme of our study which was to delineate the impact of the number of influencing variables rather than to characterize the absolute LR model performance *per se*.

The specific question we explored in our study was: "*Is Correlation Dimension is a reliable proxy for the number of dominant variables required to predict risk of arsenic contamination in groundwater by Logistic Regression?*" We considered all possible combinations of influencing variables from the total set of 11 as candidate LR models. This resulted in 2048 LR models being evaluated. Each evaluation of an LR model, pertaining to a given complexity, was repeated 25 times within the MC framework to identify the mean and the range of LR model prediction. For a given number of influencing variables, the mean of 25 MC realizations signified the most probable LR model performance while the range was an indicator of predictive uncertainty.

RESULTS AND DISCUSSION

Figure 1 shows the variation of probability of successful detection of wells, or the fraction of validation set wells correctly detected (as contaminated/uncontaminated at the 50 ppb limit) as a function of the total number of influencing variables (Table 1) in the LR model. The mean predictive ability (shown in red dotted line, Figure 1) of the LR model, while remaining insensitive to number of influencing variables in the ranges of 1 to 7 variables, was found to noticeably increase in sensitivity when the number of variables is greater than 8. A systematic reduction in the predictive uncertainty was also observed as the number of variables is increased from 8 to 11 (observe the width between the dotted lines in Figure 1). It is important to note that the predictive uncertainty (or range) has important implications for model complexity and parameter optimization. The wider the uncertainty the more challenging is the optimization for convergence to the best LR model configuration. It was observed that the predictive uncertainty increases as the LR model becomes more complex up to a total of 7 number of variables and then indicates a reverse trend from 8 to 11. We can therefore intuitively expect that model optimization is less likely to be trapped in a local optima (due to reduced predictive uncertainty) as long as model complexity exceeds 7 number of independent variables. Finally, we also observed that the best performance of the LR model occurred when the number of influencing variables is 11. This observation indicated consistency with the CD concept, where the inclusion of any additional variable deemed influential on the arsenic contamination dynamics, should yield either an improvement or simple simply no change.

Overall, our preliminary findings seem to offer credence to the hypothesis that an acceptable number of dominant variables to model the risk of arsenic contamination should range from 8-11 (or higher) as theorized *a priori* by the CD method. It should be noted, however, that more detailed studies are needed to verify the true limitations and strengths of the CD approach for building LR models for rapid assessment of risk of arsenic contamination. For example, there is a need to study the impact of noise in data on the practical utility of CD as a proxy and verify, similar to Sivakumar (2005), the impact of data size for such applications. In addition, caution needs to be exercised on the use of CD as a proxy, as it only yields a number but does not indicate the specific choice of variables and the manner in which they should be integrated in a deterministic model.

Currently, there are a number of maps available that characterize the probability of arsenic contamination in non-sampled regions based on kriging (see BGS-DPHE, 2001 and McArthur et al., 2001, for example). Preliminary findings of our study imply that an injection of the chaotic dynamic approach of LR modeling with variables equaling the CD could expedite refinement of the map towards reduction of uncertainty in risk of contamination at non-sampled locations than what would have otherwise been possible by the kriging method alone. Prior knowledge of CD as a proxy for an acceptable number of dominant variables can therefore be a valuable information that can potentially save considerable time during a rapid assessment of arsenic contamination.

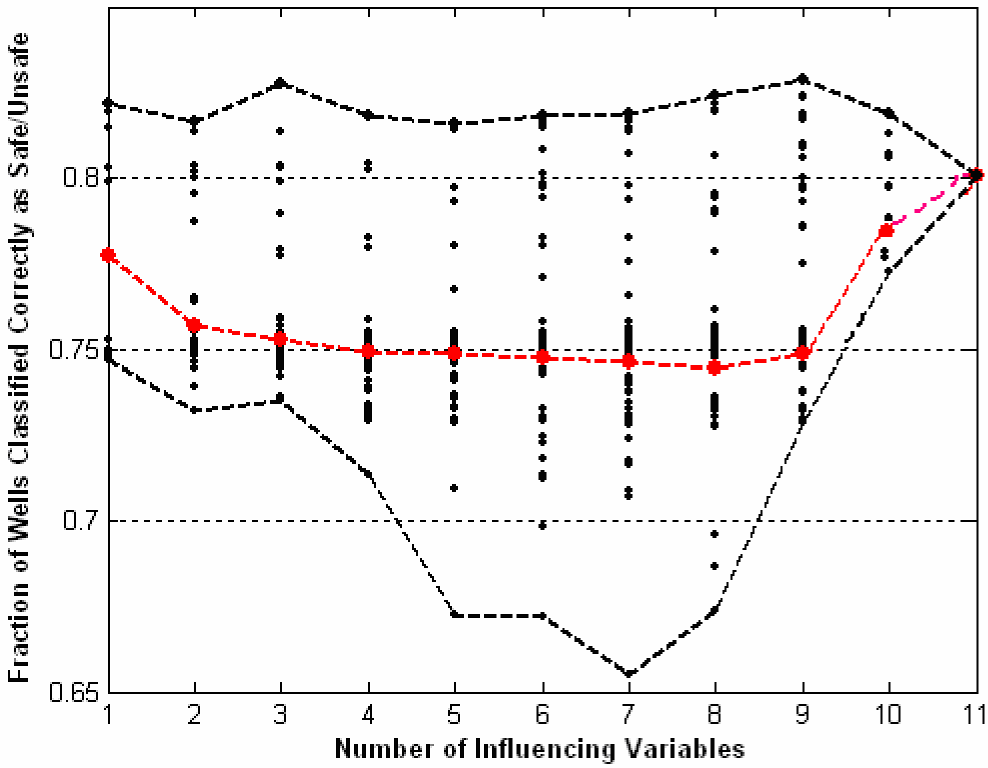

Figure 2. Variation of fraction of wells correctly classified by LR model as safe/unsafe with the number of influencing variables. Red circles indicate mean from 25 MC realizations. The dotted lines indicate the range of 25 Monte Carlo realizations for a given number of variables. Each black circle indicates a possible combination of influencing variables in an LR model of given complexity among the total of 2048 considered.

CONCLUSION

The Correlation Dimension (CD) of an attractor provides information on the number of variables present in its non-linear deterministic dynamic variability. In this study we explored the presence of a physical connection between the CD and the mathematical modeling of risk of arsenic contamination in groundwater using Logistic Regression (LR). Our database comprised a large-scale arsenic survey conducted in Bangladesh, wherein, Hossain and Sivakumar (2006) reported CD values ranging anywhere from 8 to 11 for shallow aquifers (depth < 150 m). Using 11 influencing variables that potentially dictated the variability of arsenic concentration, we have demonstrated that CD can function as a reliable proxy for the number of dominant variables required in the LR model to optimally predict arsenic contamination at non-sampled wells. Given this preliminary finding, we believe it is time we consider comprehensive investigations to assess the true merit of non-linear deterministic paradigms in conjunction with the more conventional linear stochastic methods such as kriging for reducing uncertainty of arsenic risk mapping for resources poor countries.

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