

Quantitative Calculation of Groundwater Vulnerability Assessment Based on Quantification Theory III

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Abstract: There are a lot of key qualitative variables in factors affecting groundwater vulnerability. The processing of qualitative variables of the existing superimposed index method generally relies on experience, so the results are normally subjective. Quantitative theory can handle qualitative variables quantitatively, achieve the unity of quantitative and qualitative indicators, highlight the decisive role of the main factors and reflect the actual situation more objectively. We took Yulin City as the research area to verify the feasibility and applicability of quantitative theory III, which is used for the quantitative evaluation of groundwater vulnerability. The results show that it has obvious advantage in the screening of indicators and the groundwater vulnerability partition, so it can be used as a quantitative calculation method of groundwater vulnerability assessment.

Keywords: Groundwater, Vulnerability assessment, Quantitative calculation, Quantification theory III

With the intensification of Groundwater contamination caused by human activities, aquifer point source and non-point source pollution problems have been around the world (Wei-hong ZHANG, 2007). Currently, as the basic work of groundwater pollution prevention, process simulation and contraposed index are main methods among groundwater vulnerability assessment (Yan-guo TENG, Jie SU, 2012). Contraposed index is most widely used because of its simplicity and operability, among which, DRASTIC model has been the most commonly used method for the combination of qualitative and quantitative variables. There exists different choices of factor interval division, weight assignment and antifouling performance index calculation in applying the model (Zuo-shen ZHONG, 2005), therefore, many scholars have proposed improved methods. LEI Jing determined the parameters of the scoring system by numerical simulation, E Jian determined the weight of each index by AHP and

Fuzzy Comprehensive Evaluation and YU Xiang-qian determined the weight by combination of weight distribution (Jing LEI, Si-cong ZHANG, 2003; Fang ZHANG et al., 2007; E Jian et al., 2010; Xiang-qian YU et al., 2012.). All of these have failed to achieve quantitative calculation of qualitative data.

Proposed by Hayashi Chikio, a Japanese scholar, the quantification theory is suitable for multidimensional qualitative data processing (Wen-quan DONG et al., 1979), and has been well studied in geological disasters and other research areas (Xi WANG, Guang-jie LI, 2006; Jun-xia LI et al., 2010). Quantification theory III is based on reaction matrix. In the calculation process, the scores of samples with similar reaction are similar, then we can find out the factor playing dominant role through further analysis, and achieve sample classification finally. In view of its advantage in quantitative calculation of qualitative data, we achieve the quantitative calculation of groundwater vulnerability assessment, as well as verify its

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validity and applicability through comparing with the conventional method.

Basic Theory and Data Processing Method

Quantification Theory III

In quantification theory, qualitative variables is called as "item", the "value" of the "item" is called as "category". Assuming the number of sample, item and category are n, s, m ($n=s+m$) respectively, then the original data constitutes a reaction matrix:

$$\begin{bmatrix} \delta_1(1,1) & \Lambda & \delta_1(1,r_1) & \Lambda & \delta_1(m,1) & \Lambda & \delta_1(m,r_m) & \mu_{11} & \Lambda & \mu_{1s} \\ \delta_2(1,1) & \Lambda & \delta_2(1,r_2) & \Lambda & \delta_2(m,1) & \Lambda & \delta_2(m,r_m) & \mu_{21} & \Lambda & \mu_{2s} \\ M & & M & & M & & M & M & & M \\ \delta_n(1,1) & \Lambda & \delta_n(1,r_n) & \Lambda & \delta_n(m,1) & \Lambda & \delta_n(m,r_m) & \mu_{n1} & \Lambda & \mu_{ns} \end{bmatrix} \quad (1)$$

$$\text{Which: } \delta_i(j, r_j) = \begin{cases} 1 & \text{qualitative data of } j\text{-th item of } i\text{-th sample is category } r_j \\ 0 & \text{qualitative data of } j\text{-th item of } i\text{-th sample is not category } r_j \end{cases}$$

Variable score is:

$$b = (b_{11}, \Lambda, b_{1n}, \Lambda, b_{m1}, \Lambda, b_{mr_m}, a_1, \Lambda, a_s)^T,$$

The average score of the i -th sample:

$$y_i = \frac{1}{m+s} \sum_{j=1}^m \sum_{k=1}^{r_j} b_{jk} \delta_i(j, k) + \sum_{k=1}^s a_k \mu_{ik} \quad (2)$$

Thus, the main problem of Quantification theory III is transformed into solving the vector b and y . Steps are as follows:

Firstly, calculate the average of total score of all samples. Response score of k -th category of j -th item of all Samples is: $(g_{11}, L, g_{1r_1}, L, g_{m1}, L,$

$$g_{mr_m}, \begin{pmatrix} 6 & 7 & 8 & \dots & s \\ 0 & 1 & 0 & & \end{pmatrix}),$$

Then the mean score is:

$$\bar{y} = \frac{1}{n(m+s)} g^T b \quad (3)$$

Secondly, calculate the inter-group variance and total variance.

$$\sigma_b^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2 = \frac{1}{n(m+s)^2} b^T H b \quad (4)$$

$$\sigma^2 = \frac{1}{n(m+s)} \left(\sum_{j=1}^m \sum_{k=1}^{r_j} b_{jk}^2 g_{jk} + n \sum_{k=1}^s a_k^2 \right) - \bar{y}^2 = \frac{1}{n(m+s)} b^T L b \quad (5)$$

$$H = X^T X - \frac{1}{n} g g^T; L = G - \frac{1}{n(m+s)} g g^T; = \text{diag.}$$

Finally, calculate the correlation ratio between inter-group variance and total variance.

$$\eta^2 = \frac{\sigma_b^2}{\sigma^2} = \frac{b^T H b}{(m+s) b^T L b} \quad (6)$$

$$H b = \lambda (m+s) L b \quad (7)$$

Formula 7 is the mathematical model of quantification theory III. The solution which maximize η^2 and meet the condition: $b^T L b = 1$ and $g^T b = 0$ is corresponding eigenvectors of largest eigenvalue of formula 7. Multi-dimensional is available when the one-dimensional representation is not ideal. It is seeking corresponding eigenvectors b of the first A maximum eigenvalue of formula 7.

Data Processing Method

Data processing which based on the calculation step above is a superposition of each element vector. We can get multiple independent irregular curved edge shapes, each can be considered as a computing unit, among all the values, at least one is different from other units. All the computing units compose a sample set, from which we can compute scores of each item and category, analysis the dominant component, and complete the sample

classification. Fig.1 shows the basic calculation process.

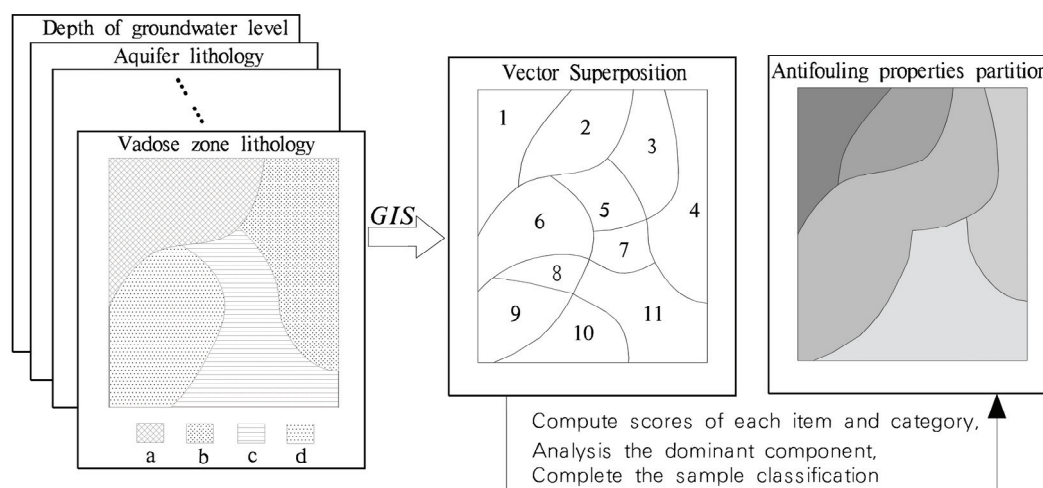


Fig.1 Process of Groundwater Vulnerability Assessment Groundwater Based on Quantification Theory III Research Case

water, water resources protection work needs to be strengthened.

Study Area

Study area is located in Yulin City, Shanxi Province, a nationwide survey of groundwater pollution investigation in 2012. Yulin is located in the bordering area of Maowusu sandy and the loess plateau, where the surface water resources is shortage, groundwater accounts for more than 60% of the total amount of water. It belongs to the semi-arid continental monsoon climate, annual rainfall is 300~550 mm. Study area includes three geomorphic types: river valley area, desert beach area and loess area (Fig.2). Pore water in river valley area and desert beach area as well as fissure water in burnt rocks area with good quality and quantity are the major source of local residents' life and production. According to the groundwater pollution investigation and sample test results in 2012, the phenomenon whose standard-exceeding of hydrochemical index is widespread where human activity is intense. Mainly as follows: "Three Nitrogen" is excessive seriously, hardness increase significantly, heavy metal pollution highlights, Fe and Mn excess in large area, as well as a series of other groundwater quality problems. Therefore, in order to ensure the safety of drinking

Factors Affecting the Groundwater Vulnerability

Considering geological and hydrogeological conditions in the study area, we choose vadose zone lithology, depth of groundwater level, aquifer lithology, water yield property and rainfall recharge coefficient as the factors to achieve groundwater vulnerability assessment. Vadose zone is a direct barrier to keep groundwater from contamination; aquifer lithology reflects hydraulic transmission capacity; water yield property determines the ability to gather water at a point, the pollution hazard results will be worse if it is stronger; rainfall recharge coefficient reflects the dynamic of vertical migration of contaminants. All these five factors cover the surface, underground and outside force of pollutant transferring into groundwater. So they can be integrated to reflect the groundwater vulnerability in study area. The rainfall recharge coefficient is a quantitative variable, others are qualitative variables. 44 calculation units are obtained by overlaying all these five vector layers (Fig.3).

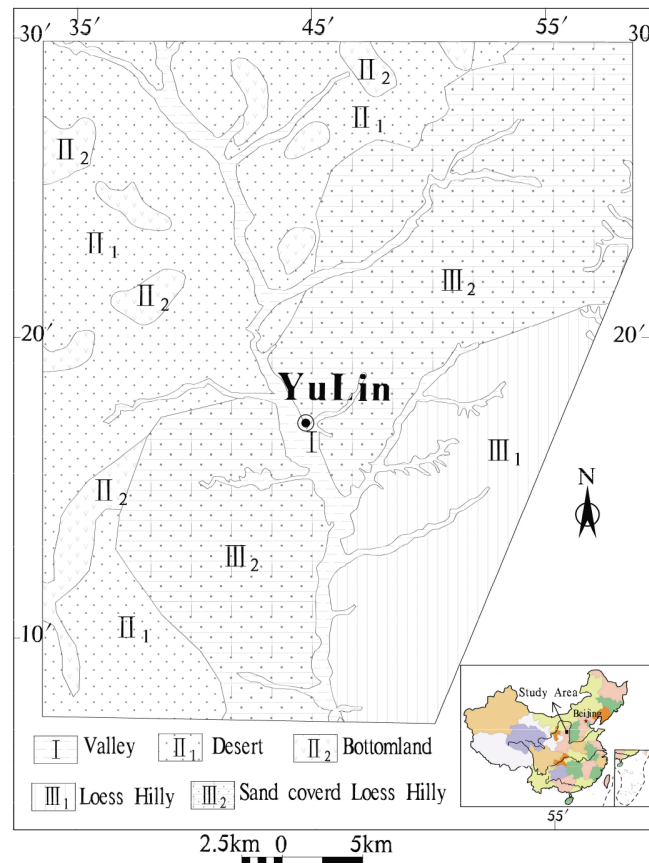


Fig.2 Topography Thumbnail of Study Area

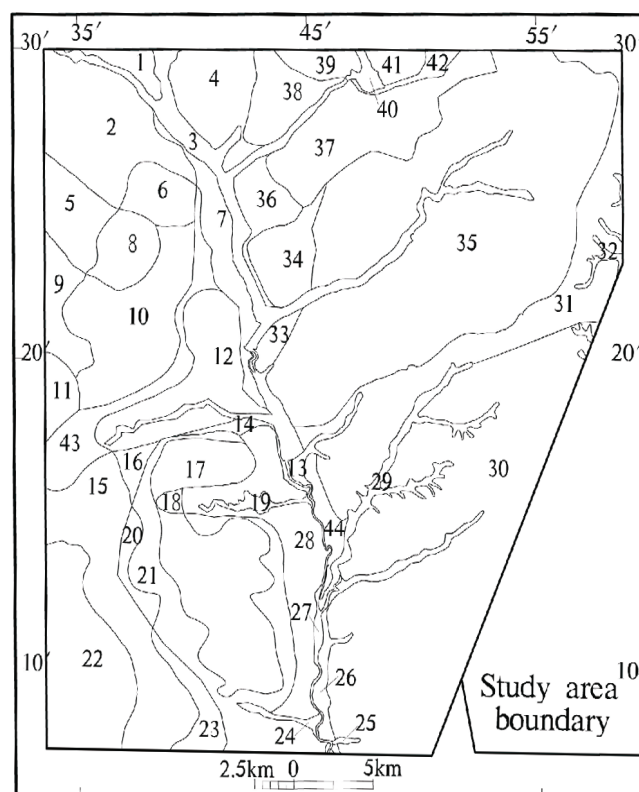


Fig.3 Divided Computing Units

Groundwater Vulnerability Assessment

According to the conditions in the study area, the above items are divided into 16 categories (Table 1). Then a reaction matrix is established in the principle of formula 2.

Based on the above calculation steps,

programming in Matlab is completed. Finally we obtain sum of corresponding correlation ratio of the form two largest eigenvalues ($\lambda_1 = 0.21$, $\lambda_2 = 0.16$) is 78%, which has been able to represent most of the information of each factor. The two largest eigenvalues and category scores are shown in Table 2.

Table 1 Criterion for the Classification of Items and Categories of Influential Factors

Item	Category Classification				
Groundwater Depth (m)	>20	8~20	5~8	2~5	<2
Aquifer Lithology	Loess	Sand and gravel			
Water Yield Property (m ³ ·d ⁻¹)	<10	10~100	100~500	500~1,000	1,000~5,000
Vadose Zone Lithology	Loess	Sand upper , lower the loess	Sand		
Rainfall Recharge Coefficient	Quantitative data				

Table 2 Groundwater Vulnerability Influential Factors Category Score

Item	Category	Category No.	b_1	b_2
Groundwater Depth (m)	>20	1	0.11	0.06
	8~20	2	0.001	0.12
	5~8	3	-0.05	0.02
	2~5	4	-0.08	0.004
	<2	5	-0.08	-0.02
Aquifer Lithology	Loess	6	0.01	0.1
	Sand and gravel	7	-0.07	0.03
Water Yield Property ($\text{m}^3 \cdot \text{d}^{-1}$)	<10	8	0.19	-0.04
	10~100	9	0.1	0.1
	100~500	10	-0.02	-0.19
	500~1,000	11	-0.04	0.02
	1,000~5,000	12	-0.04	-0.04
Vadose Zone Lithology	Loess	13	0.3	-0.27
	Sand upper , lower the loess	14	0.06	0.14
	Sand	15	-0.07	0.03
Rainfall Recharge Coefficient		16	-0.06	-0.05

The score range of each item that is shown in Table 3 determines its contribution to groundwater vulnerability assessment (Wen-quan Dong et al., 1979). Calculation formula of the score range is expressed as: $P = \max b_{jx} - \min b_{jk}$ ($1 \leq k \leq r_j$, $1 \leq j \leq m$). The order of impact on groundwater vulnerability assessment is Vadose zone >

Groundwater depth > Water yield property > Aquifer lithology > Rainfall recharge coefficient, which is roughly the same with the order of index weight used in the classic DRASTIC model. It shows that the calculated contribution based on quantification theory III is reliable. Comparing with other methods, such as the most common

used analytic hierarchy process and fuzzy mathematics, the whole calculation process is not doping of any subjective factors. So the result is absolutely objective. Considering the corresponding category score of the form two largest eigenvalue λ_1 and λ_2 as points in the plane. According to the distance from the origin of each point, contribution of the category is filtered into three types (shown in Table 4 and Fig.4). Type I ~ III represent the main categories, secondary categories and general categories respectively that affect groundwater vulnerability. The Category number of the main categories is 8

and 13 which are shown in Table 2. It means that groundwater vulnerability has been significantly improved when the vadose zone lithology is loess and water yield property is less than $100\text{m}^3/\text{d}$.

The impact on groundwater vulnerability of the selected leading projects and categories based on category score is consistent with hydrogeological conditions in study area. Furthermore it also shows that the representative eigenvalues and eigenvectors selection is reasonable and results are credible. So we can calculate sample score and complete the following classification depending on above data.

Table 3 Groundwater Vulnerability Influential Factors for Project selection

Item	Groundwater Depth	Aquifer Lithology	Water Yield Property	Vadose Zone Lithology	Rainfall Recharge Coefficient
Contribution	0.33	0.10	0.20	0.57	0.01
Order	2	4	3	1	5

Table 4 Statistics of Category Space Distance

Category No.	1	2	3	4	5	6	7	8
Distance	0.125	0.12	0.054	0.08	0.082	0.1	0.076	0.236
Type	II	II	I	I	I	II	I	III
Category No.	9	10	11	12	13	14	15	16
Distance	0.102	0.073	0.057	0.098	0.404	0.152	0.076	0.078
Type	II	I	I	I	III	II	I	I

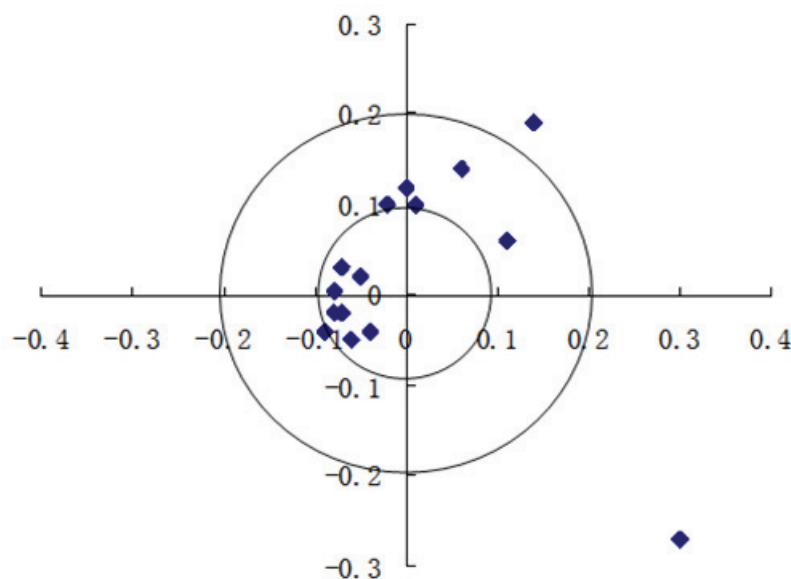


Fig.4 Spatial Categories Distribution of Groundwater Vulnerability Influential Factors

Firstly we calculate the sample score according to equation 6, and then divide the 44 samples into five classes using Q-type clustering method. Each class represents a level of groundwater vulnerability. Samples in each class are given the same colour, we can obtain groundwater vulnerability assessment chart in the study area (shown in Fig.5). Regions of poor groundwater vulnerability located in the valley area and northwest winds beach area with loose structure and small thickness of vadose zone, as well as higher hydraulic conductivity, so the contaminants can spread easily. Regions of medium groundwater vulnerability located in the sand cover loess area where the groundwater depth is larger and the vadose zone has dual structure of sand upper and

lower the loess. Regions of medium groundwater vulnerability mainly located in the southeastern Loess hilly area where the lithology is large and thickness silty loess, aquifer permeability coefficient is small. So groundwater is unlikely contaminated from outer pollutant source in this area.

Groundwater vulnerability is also calculated using contraposed index method. There exist subtle differences of border demarcation after comparing the two evaluation results. However the regional trend of groundwater vulnerability is consistent in Fig.5 and Fig.6. This also explains the result of groundwater vulnerability assessment based on quantification theory III is reasonable and credible.

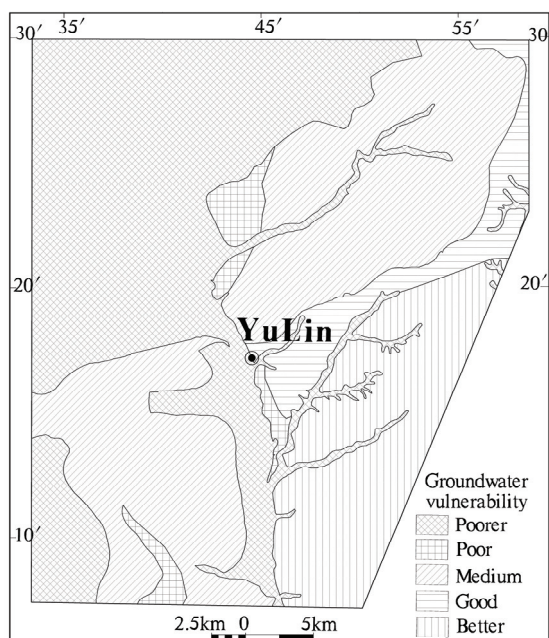


Fig.5 Assessment Based on Quantification Theory III

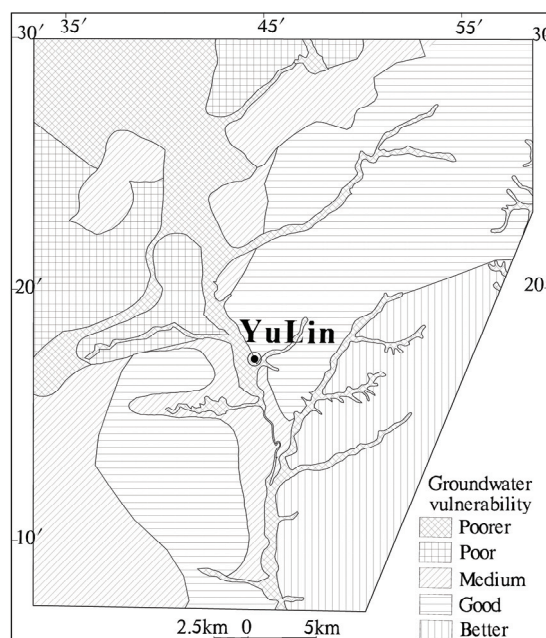


Fig.6 Assessment Based on Superimposed Index Method

Conclusions and Discussions

By taking Yulin City and surrounding areas as study area, we achieve a quantitative calculation of groundwater vulnerability assessment based on quantification theory III in this paper. It is proved that quantification theory III is an effective quantitative calculation of groundwater vulnerability assessment by comparing with the result of contraposed index method. It can quantify

the qualitative issues processing, unified qualitative and quantitative indicators. So it has two advantages as follows. The first one is indicators selecting: the weight of each indicator is calculated quantitatively from the sample data, which is different from the traditional methods that give weights firstly, and then calculate the score of each indicator, so the indicator weight is more objective. The second one is partition of antifouling performance: sample classification is obtained by clustering based on the sample score,

so it overcomes the subjectivity of the traditional methods whose part is different indicator ranges.

The accuracy of project and category classifying of the original data sample is the key point to the calculation using quantification theory III. We achieve the quantitative calculation of groundwater vulnerability assessment in this paper. However, it needs to be further improved in the aspect of category refinement so as to continuously improve its usefulness.

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