



## Research Article

# Evaluation of Water Quality by Means of Probabilistic Multi-Objective Optimization

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**Abstract:** Water quality assessment is a problem in a complex multi-attribute system, and rational approach is still in need for comprehensive evaluation. In this article, a Probabilistic Multi-Objective Optimization (PMOO) evaluation approach for water quality assessment is presented rationally. Firstly, it proposes a quantitative evaluation method of the utility value of each evaluated attribute (indicator), the integration of the utility value with the probabilistic multi-objective optimization is conducted to complete the evaluation and comparison of water quality evaluation comprehensively with a practical example from 7 sampling points of Jinchang city of Gansu province, China, to illuminate the procedure of the approach. Six performance metrics are involved, which include total salinity, total hardness, nitrite, nitrate, phenol, and hexavalent chromium. The evaluated result indicates that the sampling point 1 exhibits the highest total preferable probability and is ranked No. 1 in the comprehensive assessment of quality of water resources by means of PMOO. The proposed approach eliminates the human factors in the previous assessments for comprehensive evaluation with multiple performance metrics.

**Keywords:** water quality, comprehensive evaluation, utility, probabilistic multi-objective optimization, ranking

## 1. Introduction

Water quality assessment is a problem in a complex multi-attribute system, reasonable approach is still in need, which relates to the sustainable development in China significantly [1]. In recent years, though there have been many achievements in water quality evaluation, each of them has its essential shortcoming in addition to special advantages [2]-[8]. The details are given as follows.

### 1) Single index evaluation method

The single index evaluation method could not consider the comprehensiveness of water quality, which classifies water quality according to “one single index” completely, and might not objectively reflect the actually comprehensive situation of water quality or even lose some information, especially for comprehensive comparison.

### 2) Comprehensive evaluation model based on fuzzy mathematics

The comprehensive evaluation model based on fuzzy mathematics is a “principal factor prominent” evaluation method, it remains the so-called “principal factor” but ignores other “minor factors”. Although its calculation is intuitive and simple, it loses a lot of information and makes it difficult to provide a clear attribution of evaluation.

### 3) Grey clustering analysis method

Though the grey clustering analysis method has noticed the fuzziness of water quality grading boundaries and greatly improves the information utilization rate and accuracy, the resolution of the evaluation results is low, and sometimes it even does not match the actual situation. Besides, it involves a resolvable factor (in fact, a human factor) in the calculation of the so-called “grey correlation degree”. Finally, the criterion based on the “grey correlation degree” is irrational.

### 4) Entropy model of water quality evaluation

An entropy model of water quality evaluation was developed [3]-[9]. This approach was proposed on basis of the theory of grey system and Jaynes’ maximum information entropy principle in information theory [3]-[9]. Zhao found that there were some problems in the method of determining the grade membership between samples and evaluation criteria in the model when he used this model to study the water quality assessment [9].

Actually, in the grey system evaluation, there is also a problem of unclear parameters [10], [11], which is irrational [2], [12]-[14]. Besides, Jaynes’s probability is the probability of “rational inference” [15], not the basis of tendentious judgment. Jaynes inherited and developed the idea of statistical mechanics from physicist Gibbs, and systematized it into the “the maximum entropy principle”, thus he took it as the basic point. Jaynes’s concept of probability can be summarized as follows: a) its essence is logical and subjective (cognitive). Jaynes believed that probability is not the inherent property of objective things (as the frequency school thinks) [15], but the quantification of the degree of confidence in the rationality of propositions based on existing knowledge. It is a reasoning tool, which is used to make the most reasonable and impartial inference under the condition of incomplete information; b) the core of the methodology is maximum entropy of the system. The principle of maximum entropy is its starting point. When we are faced with some information (constraints), we should choose the one state which is with the largest entropy among all the probability distributions that may satisfy these constraints. Because this distribution adds the least “subjective assumptions”, it is the fairest and most stable choice. It represents the “maximum uncertainty” under the known information and avoids any arbitrary presupposition of unknown information; c) the explanation of “probability” here is a measure of cognitive uncertainty. For example, given that the average value of a dice is 4.5, the maximum entropy principle will infer the probability distribution of each face, which reflects the cognitive state of “we don’t know whether the dice are fair or not”, rather than the physical properties of the dice itself; d) the purpose of the story is to carry out the best and most unbiased reasonable prediction on basis of limited information. All these contents only indicates that Jaynes’s probability is the probability of “rational inference”, which could not a basis of any tendentious judgment.

### 5) Potential regulation by means of probabilistic multi-objective optimization

Recently, a Probabilistic Multi-Objective Optimization (PMOO) methodology is proposed, which introduces a new concept of “preferable probability” to reflect the preference degree of an objective in the optimization problem [12]-[14]. In PMOO [12]-[14], the concept of “preferable probability” was deeply inspired by Jaynes’s thought, but it was purposefully transformed, and its application field was specialized. The main idea of PMOO can be summarized as follows: a) the essence is decision-making and functional, especially for comprehensive comparison. “Preferable probability” is put forward to solve a core problem in multi-objective optimization: how to scientifically and quantitatively integrate the subjective preference of Decision Makers (DM) into the optimization process. It quantifies the possibility that a solution (or target vector) is “preferable” or “selected” by decision makers; b) the core of the methodology is to construct a probability based on utility of attributes; c) the explanation of “probability” here is no longer pure cognitive uncertainty, but the quantification of “choice tendency” which combines subjective preferences. The question it answers is: “Given the preference of the decision maker, how likely is he/she to choose this solution?”; d) the purpose of qualitative “preference” is to transform it into a strict and computable “probability distribution”, so that the multi-objective optimization problem can be transformed into a single-objective optimization problem that can be searched efficiently based on probability, for example, to find the solution with the highest probability of preference.

To get a better understanding, we can use a metaphor as follows.

A). As to Jaynes’s probability, it is like the “weather forecast”. The Meteorological Observatory calculated that “the probability of rain tomorrow is a certain value (says 45% for example)” according to historical data and models. This is an estimation of the uncertainty of the objective natural phenomenon (rain). It does not include any subjective preference of “I like rain” or “rain is better”; B). As for the preferable probability in PMOO, it is like the “score of a beauty contest”. The judges graded each player according to his appearance, talent, and other indicators (goals). Finally,

we convert all the judges' scores into a comprehensive score through a rule and normalize it to a percentage form. "Player A's preferable probability is some value (says 80% for example)" does not mean that he/she is likely to be an individual exactly at the corresponding value, but means that under the current judges and grading standards, he/she is more preferable than other players. This probability value is especially constructed for ranking and decision-making.

The above discussions indicated that PMOO is more proper for water resource quality evaluations with multiple attributes, particularly for comprehensive comparison and ranking.

The aim of this paper is to present an integration of the utility value with the probabilistic multi-objective optimization to conduct water resources quality comprehensively.

## 2. Outline of PMOO

### 2.1 Main idea of PMOO

Because the original intention of Multi-Objective Optimization (MOO) is "simultaneous optimization" of multiple objectives in a system, it can establish an appropriate method only by taking this intention into account [12]-[14].

From the perspective of probability theory, it is the "product" of the probabilities of all attributes, i.e., the "joint probability" in the language of probability theory, while it belongs to the "intersection" of all attributes in set theory. In addition, in order to make the problem operable in PMOO, a new concept of "preferable probability" is introduced to address the preference degree of an attribute of an alternative candidate in the optimization.

Due to the special function of preferable probability, the "probability of preference" is used to quantify the credibility of "overall superiority" between two multi-objective solutions in PMOO. The following are its core points [12]-[14]:

#### 1. Essence

The complex comparative relationship between two multi-objective solutions (high-dimensional vectors) is compressed into a scalar value by probability tools to measure the probability that "solution *A* is better than solution *B*". For example, in the multi-objective optimization problem, if solution *A* performs better on multiple objectives, its "preferable probability" will be higher.

#### 2. Evaluation method

The value of preferable probability is a numerical value between 0 and 1, which is directly related to the utility value of the corresponding attribute linearly, its exact correlation depends on the preference to the corresponding utility value of the attribute in the optimization process.

#### 3. Function

It provides a more flexible solution sequencing and decision-making basis, especially when the Pareto dominance relation in traditional multi-objective optimization fails in high-dimensional space. For example, in engineering design, resource allocation, and other scenarios, it can help to quickly screen better multi-objective solutions.

#### 4. Difference from traditional probability

The preferable probability is an artificially constructed tool, particularly for preference measurement, which is used to compare solutions in multi-objective optimization and reflects subjective preference or competitiveness. While Shannon's probability is usually used to measure the objective possibility (likelihood) of random events, such as the probability of rain in a weather forecast.

In summary, the "preferable probability" is an innovative application of probability theory in the field of multi-objective optimization, which aims to provide a quantitative basis for complex decision-making by solving the relationship between advantages and disadvantages through probability language.

The evaluation objectives (attributes) of candidate schemes in optimization tasks are preliminarily divided into two basic types in PMOO: i.e., both beneficial type of attributes and unbeneficial (cost) types of attributes, quantitative evaluations of partial preferable probability corresponding to both beneficial attributes and unbeneficial (cost) attributes are formulated [11]-[13]. Furthermore, it takes the "simultaneous optimization of multiple attributes" as the overall optimization of a system; the total preferable probability of each candidate is the product of partial preferable probabilities of all possible attributes of the candidate scheme. Starting from simplicity, it is also assumed that each partial preferable probability is linearly positively correlated with the utility index of its beneficial attributes, and each

partial preferable probability is linearly negatively correlated with the utility index of its unbeneficial attributes [12]-[14]. Finally, the total preferable probability of each candidate scheme is the uniquely decisive index for the candidate scheme to win this optimization competition.

The procedure of PMOO evaluation is shown in Figure 1 [12]-[14].

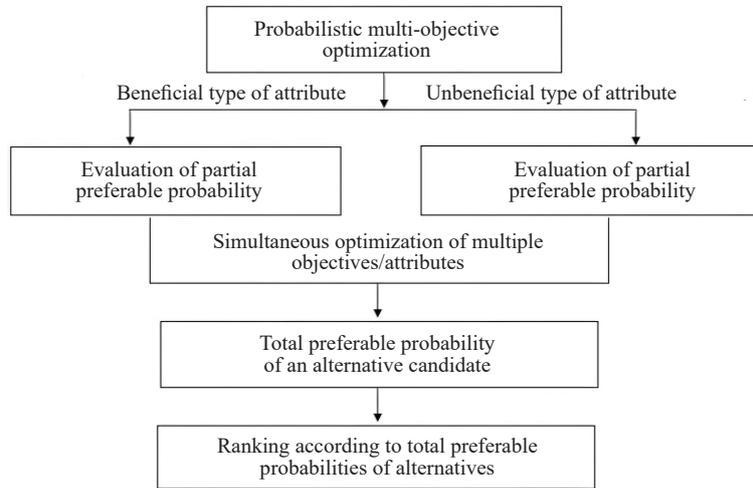


Figure 1. Evaluation procedure of the PMOO method

## 2.2 Formulations in PMOO evaluation

1) Evaluation of partial preferable probability in case of a beneficial type of attribute is expressed in Eq. (1) [12]-[14],

$$P_{ij} = A_j Y_{ij}, A_j = 1/(k\bar{Y}_j), i = 1, 2, \dots, k; j = 1, 2, \dots, l. \quad (1)$$

2) Evaluation of partial preferable probability in case an unbeneficial type of attribute is presented in Eq. (2) [12]-[14],

$$P_{ij} = B_j (Y_{j\max} + Y_{j\min} - Y_{ij}), B_j = 1/[k(Y_{j\max} + Y_{j\min} - \bar{Y}_j)],$$

$$i = 1, 2, \dots, k; j = 1, 2, \dots, l. \quad (2)$$

3) Total preferable probability of an alternative candidate is given in Eq. (3) [7]-[9],

$$P_i = P_{i1} \cdot P_{i2} \cdots P_{il} = \prod_{j=1}^l P_{ij}, i = 1, 2, \dots, k; j = 1, 2, \dots, l. \quad (3)$$

In Eq. (1) through Eq. (3),  $P_{ij}$  reflects the preferable probability of the  $j$ -th performance attribute of the  $i$ -th alternative [12]-[14],  $k$  is the total number of alternative candidates, and  $l$  is the total number of performance attributes;  $P_i$  indicates the total preferable probability of the  $i$ -th candidate;  $Y_{ij}$  reflects the utility index value of the  $j$ -th performance attribute of the  $i$ -th alternative candidate;  $A_j$  is the normalization factor of the  $j$ -th beneficial type of performance attributes index;  $B_j$  reflects the normalization factor of the  $j$ -th unbeneficial type of performance attribute index;  $\bar{Y}_j$  is the arithmetic average value of  $j$ -th utility index of the performance attribute in the evaluated group;  $Y_{j\min}$  and  $Y_{j\max}$  represent the minimum and maximum values of the utility index  $Y_{ij}$  of the  $j$ -th objective in the evaluated group, respectively.

If one indicator is enhanced, the Eq. (4) for total preferable probability assessment could be used,

$$P_i = P_{i1}^{w_1} \cdot P_{i2}^{w_2} \cdots P_{il}^{w_l} = \prod_{j=1}^l P_{ij}^{w_j}, \quad i = 1, 2, \dots, k; j = 1, 2, \dots, l. \quad (4)$$

In Eq. (4)  $w_1, w_2, w_j$  and  $w_l$  indicates weighting factors of the corresponding attribute.

Besides, the evaluations of normalization factors  $A_j$  and  $B_j$  are obtained from the general principle of normalization of probability theory for  $P_{ij}$  over all alternative candidates  $i$  [12]-[14], i.e.,

$$\sum_{i=1}^k P_{ij} = \sum_{i=1}^k A_j Y_{ij} = 1, \quad (5)$$

and

$$\sum_{i=1}^k P_{ij} = \sum_{i=1}^k B_j (Y_{j\max} + Y_{j\min} - Y_{ij}) = 1. \quad (6)$$

Thus, it leads to the following results for normalization factors  $A_j$  and  $B_j$  [12]-[14],

$$A_j = 1/(k\bar{Y}_j), \quad (7)$$

and

$$B_j = 1/[k(Y_{j\max} + Y_{j\min} - \bar{Y}_j)]. \quad (8)$$

As to tackling MOO, the PMOO emphasize the simultaneity of the multiple attributes in the optimization process of a system, and the irreplaceability of each attribute. Therefore, it is analogical to the “intersection” in set theory and “joint probability” of two independent events in probability theory, which is against to any type of “additive algorithm”, accordingly a new concept of “preferable probability” is proposed, and the corresponding evaluations were formulated. However, in traditional methods for MOO evaluations, such as the Simple Additive Weighting (SAW) method, the additive algorithm is applied to the weighted attribute; obviously, this kind of “additive algorithm” contradicts to irreplaceability of each attribute. Therefore, in principle, PMOO conforms to the essence of MOO properly.

The remarkable feature of this PMOO method is to optimize multiple objectives in a system at the same time in terms of preferable probability, which is without any subjective or artificial scaling factor, and opens up a new way to solve MOO problems with broad application prospects [6]-[8]. Here, “subjective or artificial scale factor” means that it is unnecessary to introduce any nonobjective factor artificially in general cases, but it is not absolutely to repel a necessary subjective factor in special cases.

Actually, PMOO gained many applications in some fields, such as material selection, shortest path, engineering, experimental design, medical scheme, robust design of industrial processes and products, planning problems, investment optimization and so on. The possible limitation of the PMOO approach might be a lack of the introduction of modern searching methods, which affects the computational efficiency, adaptability to high-dimensional data, and accuracy in large-scale samples.

### 3. Evaluation of water quality in terms of PMOO

In this section, the approach of evaluation of water quality is conducted with one example quantitatively to illuminate the procedure of the approach. The data of the example is from literatures [2], [9], [10].

Table 1 shows a set of water quality monitoring data from literatures [2], [9], [10], which was conducted from 7 sampling points of Jinchang city of Gansu province, China [2], [9], [10]. While the evaluated standard for water quality

grading is from literatures cited in Table 2 [2], [9], [10].

**Table 1.** A set of water quality monitoring data from literatures [2], [9], [10]

Sampling point	Total salinity, mg/L	Total hardness, mg/L	Nitrite, mg/L	Nitrate, mg/L	Phenol, mg/L	Hexavalent Chromium, mg/L
1	502	25.30	0	3.15	0	0.005
2	800	23.34	0	2.30	0.002	0.003
3	782	35.44	0.140	9.30	0.002	0.010
4	1,390	73.92	0	3.05	0	0.032
5	386	17.12	0.060	3.07	0.003	0.006
6	1,385	63.01	0	12.33	0.003	0.012
7	850	35.90	0.090	17.90	0	0.147

**Table 2.** Standard for water quality grading from literatures [2], [9]

Grade	Total salinity, mg/L	Total hardness, mg/L	Nitrite, mg/L	Nitrate, mg/L	Phenol, mg/L	Hexavalent Chromium, mg/L
1	400	10	0.035	2.5	0.001	0.002
2	1,000	25	0.1	10	0.002	0.05
3	3,000	100	0.4	50	0.01	0.20

According to the general rule of “single index evaluation method” for water quality grading assessment [1]-[3], [9], [10], the evaluations for each sampling point can be conducted directly, the results are shown in Table 3.

However, as can be seen from Table 1 that there is an obvious difference among the data of sampling points, but the assessed results by means of “single index evaluation method” for water quality grading assessment could not realize it. Therefore, the evaluation result in Table 3 looks rough obviously, which could be refined further. Therefore, a new approach is needed.

**Table 3.** Evaluated results for the water quality monitoring data according to the general rule of “single index evaluation method” for water quality grading assessment

Sampling point	1	2	3	4	5	6	7
Grade	2	2	3	3	3	3	3

### 3.1 Introduction utility value for each water quality monitoring data

The utility value for each water quality monitoring data is introduced in this paper to reveal the closeness of each monitoring performance index to its corresponding critical value in the standard for water quality grading.

In order to refine the evaluation method for water quality, we could introduce a new index “utility value” for each

water quality monitoring data. The “utility value” reflects the utility of each water quality monitoring data as compared to the critical value of the standard for each attribute or index in the corresponding grade. The following procedure is to illuminate the quantification of “utility value” for each water quality monitoring data according to the following procedure:

1. For a water quality monitoring data, if its value is smaller than the corresponding critical value of “grade 1”, its “utility value” is defined as “1”;
2. If the value of water quality monitoring data is between the corresponding critical values of “grade 1” and “grade 2”, its “utility value” can be evaluated by,

$$U_{ij} = 0.5 \cdot [1 + (S_{ijc2} - S_{ij}) / (S_{ijc2} - S_{ijc1})]. \quad (9)$$

In Eq. (9),  $S_{ij}$  is the actual value of the water quality monitoring data,  $S_{ijc2}$  and  $S_{ijc1}$  indicate the critical values of the corresponding index in grade 2 and grade 1 from the standard;

3. If the value of water quality monitoring data is between the corresponding critical values of “grade 2” and “grade 3”, its “utility value” can be evaluated by,

$$U_{ij} = 0.5 \cdot [(S_{ijc3} - S_{ij}) / (S_{ijc3} - S_{ijc2})]. \quad (10)$$

4. If the value of water quality monitoring data is greater than the corresponding critical value of “grade 3”, its “utility value” is defined as “0”.

In Eq. (10), again  $S_{ij}$  is the actual value of the water quality monitoring data, similarly  $S_{ijc3}$  and  $S_{ijc2}$  indicate the critical values of the corresponding index in grade 3 and grade 2 from the standard.

Figure 2 illuminates the “utility value” of the water quality monitoring data  $S_{ij}$ .

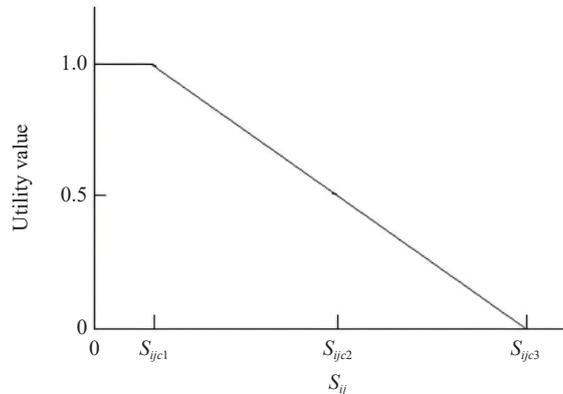


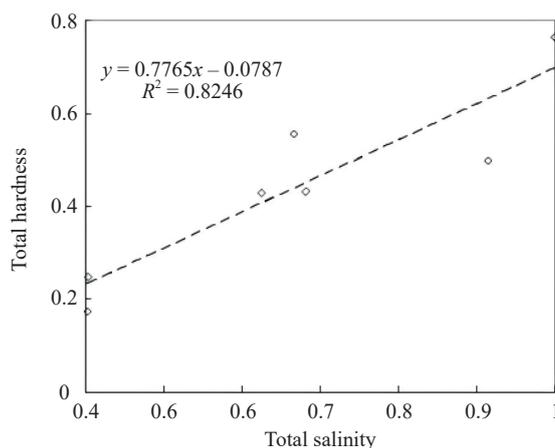
Figure 2. Illumination of “utility value” of water quality monitoring data  $S_{ij}$

Subsequently, the evaluation of the utility value of the water quality monitoring data in Table 2 can be conducted according to Eq. (9) and Eq. (10), which is shown in Table 4.

The independence of attribute utilities is discussed as follows.

The linear correlation factors of the actual utilities of total salinity, total hardness, nitrite, nitrate, phenol, and hexavalent chromium in Table 4 are presented.

Figure 3 shows the correlation between total salinity and total hardness, which shows a strong correlation with  $R_{TS-th} = 0.9081$ , therefore in the PMOO assessment one index from both total salinity and total hardness could be selected to participate in the evaluation, here in our study the total salinity is remained. In addition, the correlation between Nitrite and Nitrate is sensitive but no too high with  $R_{N-N} = 0.6010$ , therefore in the PMOO assessment, they could participate in the evaluation all together. All the other indexes have only very weak and negligible correlations.



**Figure 3.** Correlation between total salinity and total hardness

**Table 4.** Evaluated results of the utility value of the water quality monitoring data

Sampling point	Utility value of the evaluated index $U_{ij}$					
	Total salinity	Total hardness	Nitrite	Nitrate	Phenol	Hexavalent chromium
1	0.9150	0.4980	1.0000	0.9567	1.0000	0.9688
2	0.6667	0.5553	1.0000	1.0000	0.5000	0.9896
3	0.6817	0.4304	0.4333	0.5467	0.5000	0.9167
4	0.4025	0.1739	1.0000	0.9633	1.0000	0.6875
5	1.0000	0.7627	0.8077	0.9620	0.4375	0.9583
6	0.4038	0.2466	1.0000	0.4709	0.4375	0.8958
7	0.6250	0.4273	0.5769	0.4013	1.0000	0.1767

### 3.2 Evaluation of water quality by means of PMOO

Furthermore, the evaluation of water quality can be conducted by the approach of integration of utility value for water quality monitoring data with PMOO.

Since the utility of water quality monitoring data has the characteristic of the higher the better, which is a beneficial type of attribute typically, therefore the evaluation of partial preferable probability of all utilities of the evaluated indexes can be performed according to beneficial type of attribute.

Table 5 gives the evaluated results of the water quality monitoring data by means of PMOO. Table 5 shows that sampling point 1 exhibits the highest total preferable probability, therefore sampling point 1 is ranked No. 1 in the comprehensive assessment of quality of water resources by means of PMOO, which is followed by sampling point 2. It is worth mentioning that in the total preferable probability assessment, the partial preferable probability of total hardness is ignored due to its strong correlation with total salinity.

Zhao gave a difference between each sample and evaluation standard from their study [9], which showed the difference between sampling point 1 and grade 1 is the smallest with the entropy approach by chance, see Table 6. It implies that sampling point 1 gains the best position, which indicates the validation of our approach in one aspect.

**Table 5.** Evaluation results of the water quality monitoring data by means of PMOO

Sampling point	Partial preferable probability of evaluated index $P_{ij}$						Total preferable probability	Rank
	Total salinity	Total hardness	Nitrite	Nitrate	Phenol	Hexavalent chromium	$P_i \leftarrow 10^4$	
1	0.1949	0.1609	0.1719	0.1805	0.2051	0.1732	2.1482	1
2	0.1420	0.1795	0.1719	0.1887	0.1026	0.1769	0.8360	2
3	0.1452	0.1391	0.0745	0.1031	0.1026	0.1639	0.1875	6
4	0.0857	0.0562	0.1719	0.1817	0.2051	0.1229	0.6747	4
5	0.2130	0.2465	0.1388	0.1815	0.0897	0.1713	0.8245	3
6	0.0860	0.0797	0.1719	0.0888	0.0897	0.1602	0.1886	5
7	0.1331	0.1381	0.0992	0.0757	0.2051	0.0316	0.0648	7

**Table 6.** Difference between each sample and evaluation standard [9]

Grade	Sampling point						
	1	2	3	4	5	6	7
1	0.0063	0.0077	0.0256	0.0377	0.0068	0.0564	0.0924
2	0.0185	0.0121	0.0106	0.0524	0.0173	0.0386	0.0396
3	0.9752	0.9802	0.9638	0.9099	0.9759	0.9050	0.8680

### 3.3 Discussion on the evaluation result

The evaluated results shown in Table 5 indicate that sampling point 1 is positioned in No. 1, and all other sampling points are at the back of the line subsequently. In order to understand this result, let's look at the water quality monitoring data in Table 1 and Table 2 for the corresponding utility values again. It reveals clearly that the utility values of water quality monitoring data of both sampling point 1 are better than other data in many aspects comprehensively, which confirms the evaluated results. Actually, the utility values of water quality monitoring data are comparative results of water quality monitoring data with the standard for water quality grading comprehensively. Furthermore, the utility values of water quality monitoring data are integrated with PMOO to complete a comprehensive assessment of the quality of water resources, therefore such an approach is more reasonable.

## 4. Potential study in future

The approach proposed in this paper is only validated with one set of water quality data till now. In order to confirm its reasonability, more scenarios, such as varying numbers of evaluation indicators (e.g., adding pH or dissolved oxygen), and different water body types (e.g., surface water, groundwater, or seawater), etc., are still open to be studied [16]-[19].

## 5. Conclusion

The probabilistic multi-objective optimization based approach for water quality evaluation proposed in this paper by the integration of utility degree quantification with PMOO has the characteristics of clear physical concept, simplicity, and practicality reasonably, which overcomes the human factors in the previous methods. The new approach can reveal the characteristics of water quality at the sampling point as a whole comprehensively, which is not only suitable for water quality evaluation but is expected to be used in other fields. It provides a new approach for comprehensive comparison of water quality relatively, and its practical implications for water managers or policymakers can be obtained in their practical uses.

## Conflict of interest

The authors declared that there is no interest competing involved.

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