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Wine Evaluation Method Considering Physical and Chemical Indicators and Aromatic Substances

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***Abstract* – In actual life, the evaluation of wine mainly adopts the traditional sensory evaluation method, that is, by hiring some qualified wine tasters for evaluation. However, the physical and chemical indicators and aromatic substances of wine and wine grapes also have an impact on the evaluation of wine quality. Therefore, based on the quality of wine and the physical and chemical indicators of wine grapes, this paper studies the establishment of wine evaluation model, and uses K-means cluster analysis method, relative Euclidean distance weighting model and Monte Carlo algorithm to solve related problems. Solve the wine, so that the wine is divided into three levels of excellent, good and bad.**

***Keywords* – *P*hysical and Chemical Indicators, Aromatic Substances, K-means Clustering Analysis, Euclidean Distance Weighting, Monte Carlo Simulation.**

I. THE INTRODUCTION

With the development of the economy and the improvement of people's living standards, the demand for wine is also increasing, and more and more people are paying more and more attention to the quality of wine. The evaluation of wine quality is a very complicated process. When determining the quality of wine, it is generally done by hiring a group of qualified wine tasters. Each wine drinker scores the classification index after tasting the wine, and then sums it to get the total score to determine the quality of the wine. However, the quality of wine grapes is directly related to the quality of the wines produced. The physical and chemical indicators of wine and wine grape detection will reflect the quality of wine and grapes to some extent. Therefore, the industry has been trying to use the physical and chemical indicators of wine grapes and wine to evaluate the quality of wine.

This paper takes the data of the 2012 National College Students Mathematical Modeling Contest A as the source[1], and uses the normalization method to convert the secondary indicators in the physical and chemical indicators into the first-level indicators to achieve the unity of physical and chemical indicators. In the establishment of the wine grape grading evaluation model, each indicator was divided into three grades of excellent, good and bad by K-means classification method, which was rated as the physical and chemical index of wine grapes. Due to the randomness of the K-means classification method, the Monte Carlo simulation method is used to enhance the stability of the evaluation results. In addition, the quality of the wine is an important indicator of the quality of the wine grapes. First, consider the physical and chemical indicators of grapes, the quality of wine, and establish a relative Euclidean distance weighted model of wine grape rating. Then consider the effect of aromatics on the aroma of the wine, and also use the relative Euclidean distance weighted model to rank the wine grapes.

II. THE MODEL BUILDING

A. *Data Processing*

a. *Classification of Physical and Chemical Indicators* [2]

According to common knowledge and related data, physical and chemical indicators can be divided into two categories: physical indicators and chemical indicators [3]. Chemical indicators can be divided into four categories: beneficial indicators, harmful indicators, appropriate indicators, and irrelevant quantities.

b. *Classification of Aromatic Substances* [4]

The aromatic substances are all organic compounds. Since the grapes are natural products, the grape varieties determine the natural aroma of the wine. Grape and wine aromas are composed of hundreds of volatile compounds. The ingredients are very rich and complex. The main components are esters, alcohols, terpenes, phenols, acetals, lactones, fatty acids, monoterpene oxides, etc. The difference in concentration is large. Therefore, the classification of aromatic substances is mainly based on their chemical toxicity and odor, and they are classified into beneficial compounds, harmful compounds, and unrelated compounds.

c. *Normalization of Secondary Indicators*

Some physical and chemical indicators in the data have two levels of indicators in addition to the first level indicators. The second level indicators can more comprehensively display the physical and chemical characteristics of the samples than the first level indicators. Therefore, for the items with secondary indicators, the secondary indicators should be normalized. Process and use the processed secondary indicators to replace the original primary indicators.

d. *Weights of Physical and Chemical Indicators and Wine Quality*

Because the chemical index of the grape is equivalent to the taste of the wine, the taste factor accounts for 44% of the wine quality evaluation. Therefore, the weight of physical and chemical indicators and wine quality is calculated as follows:

$$\omega_1 = \frac{44}{100+44} = 0.31 \qquad \omega_2 = \frac{100}{100+44} = 0.69$$

In the middle ω_1 indicates the weight of physical and chemical indicators, ω_2 indicates the weight of the wine quality.

B. *Model of Clustering Center for Physical and Chemical Indicators and Wine Quality* [5]

There is a certain standard for ranking, and this standard should have a good degree of discrimination. Here, the K-means algorithm is used to establish clustering centers with different levels of indicators, and these cluster centers are used as the criteria for ranking.

(1) The K-means algorithm is a clustering algorithm that performs clustering based on the mean of clustering.

Input: The number of clusters k, and the algorithm of the n data objects contained.

Output: k clusters that meet the minimum variance criteria.

(2) Process flow:

① Arbitrarily select k objects from n data objects as the initial cluster center;

② Loop Step3 to Step4 until each cluster no longer changes;

③ According to the mean value (center object) of each cluster object, calculate the distance between each object and these center objects, and re-divide the corresponding objects according to the minimum distance;

④ Recalculate the mean (center object) of each (with change) cluster.

(3) Working process of K-means algorithm [6]

Step 1 arbitrarily select k objects from n data objects as the initial cluster center.

Step 2 assigns objects outside the cluster center to their most similar clusters (represented by the cluster center) according to their similarity (distance) with these cluster centers.

Step 3 calculates each cluster center obtained (the mean of all objects in the cluster).

Step 4 Repeat Step1 to Step3 until the standardization function starts to change.

The mean square error is generally used as a standard function, which is defined as follows:

$$E = \sum_{n=1}^{k} \sum_{p=c_i} \left| p - \mathbf{m}_i \right|^2 \tag{1}$$

Where E is the sum of the mean squared deviations of all objects in the database, and p is a point in the space representing the object, m_i For the mean of clustering (p and m_i Both are multidimensional).

The clustering standard shown in formula (1) is intended to make the obtained k clusters have the following characteristics: each cluster is as compact as possible, and separate clusters as much as possible.

C. *Establish a Model for Evaluation of Wine Grape Grades*

The grape grade is determined by calculating the sample index and the Euclidean distance of the cluster center, and weighting the Euclidean distance of the physical and chemical indicators and the Euclidean distance of the wine quality. Euclidean distance between the physical and chemical indicators and the Euclidean distance weight of the wine quality d_k after that, take the minimum value, where k is the grade of this grape. Based on this, the expression of the wine grape rating is:

$$\begin{cases} \min\left[d_k\right] \\ d_k = \omega_1 \dfrac{\sqrt{\sum_{i=1}^{n} \left(\dfrac{C_{ij} - C'_{ik}}{C'_{ik}} \right)^2}}{n} + \omega_2 \sqrt{\left(\dfrac{G_j - G'_k}{G'_k} \right)^2} \end{cases} \tag{2}$$

(2) where i = 1, 2, 3...n denotes n-type physical and chemical indicators, k = 1, 2, 3 respectively correspond to three levels of excellent, good and bad, j =1, 2, 3... 27 indicates the number of the red grape sample. When studying white grapes, j = 1, 2, 3...28 indicates the number of the white grape sample. C_{ij} Showing the physical and chemical indicators of the grape sample, C'_{ik} a clustering center representing the i-th physical and chemical index, G_j Indicates the quality of the wine produced by the grape sample, G'_k a clustering center that represents the quality of wine, d_k a weighted sum of the Euclidean distances of the cluster centers representing the grapes.

Whenever a grape sample is given according to the above expression, a minimum can be obtained. d_k at this time, k is the grade of the grape.

D. *Model for Determining the Grade of Grapes when Considering the Aromatics in Wine Grapes*

To consider the influence of aromatic substances on the grape grade, it is only necessary to treat the indicators of the aromatic substances in a certain way, and the introduction of the previous model is sufficient. The aromatic substances are classified. When the model is introduced, the beneficial compounds are treated as beneficial indicators, the harmful compounds are treated as harmful indicators, and the unrelated compounds are treated as irrelevant amounts to obtain clustering centers of various levels of aromatic substances. Then the data of the aromatic substance is added to the original model as a physical and chemical index, and the new model obtained is a grape classification model considering the aroma of the wine grape.

After the introduction of the indicator of aromatic substances, the structure of the data has changed, so the weight of physical and chemical indicators ω_1 and the weight of the wine quality ω_2 it should be recalculated.

Aromatic substances mainly affect the wine's aroma, taste factor and aroma factor of 74% of the total, so the weight of physical and chemical indicators and wine quality is recalculated as follows:

$$\omega_1' = \frac{44+30}{100+44+30} = 0.43 \qquad \omega_2' = \frac{100+30}{100+44+30} = 0.57 \tag{3}$$

ω_1 indicates the weight of physical and chemical indicators, ω_2' indicates the weight of the wine quality.

III. The Model Solution

A. *Method of Model Solving*

Step 1 Introduce the physical and chemical indicators of the grape samples to be rated and the wine quality data into the model.

Step 2 Process the imported data according to the classification and processing methods of the indicator.

Step 3 Introduce the various data obtained in the second step into the model of 2.3 to obtain the grade of the grapes to be tested.

If you consider the effects of aromatics in wine grapes, simply import the data from the aromatics and re-run Step 1 to Step 3 will do.

B. *Guaranteed Grading Stability Method*

Due to the randomness of the K-Means algorithm, the cluster center obtained each time is random, which leads to the randomness of the model results. This randomness is expressed in the multiple grading of the same grape sample. The result is instability, and in short, there are differences in the results of multiple grading. Too much instability is obviously unreasonable, so to reduce this instability, the Monte Carlo algorithm is used here to reduce this randomness.

a. *Monte Carlo Algorithm*

The Monte Carlo algorithm is a computational method based on probabilistic and statistical theoretical methods. Statistical simulation Method, which refers to the use of random numbers (or more common pseudo-random numbers) to solve many computational problems, it is to associate the solved problem with the same fixed probability model, and use computer to implement statistical simulation or sampling to get an approximate solu-

-tion to the problem.

The basic idea of the Monte Carlo algorithm is that when the solution to the problem is the probability of an event, or the mathematical expectation of a random variable, or the amount associated with it, is derived from some experimental method. The probability of occurrence of the piece, through which it gets the solution to the problem. Simulate a huge number of random trials by computer. The process can effectively reduce the instability of the model and improve the stability of the grape classification.

b. *Classification of Wine Grapes*

(1) *Using Monte Carlo Algorithm to Reduce Model Instability*

Each grape sample was graded 100 times according to the requirements of the Monte Carlo algorithm, and the grades of each grape were obtained by analyzing the probability data obtained. The probability that each grape falls on each level is as follows:

Table 1. Probability of wine grape grading at each level.

Grape number		1	2	3	4	5	6	7	8	9	10
	Excellent	1	1	1	0	0	0	0	0	1	1
Red grapes	Good	0	0	0	0	1	1	1	0	0	0
	Difference	0	0	0	1	0	0	0	1	0	0
	Excellent	0.38	0	0.38	0.38	0.38	1	0	0.38	0	0.38
White grape	Good	0.62	1	0.62	0.62	0.62	0	0.55	0.62	0.49	0.62
	Difference	0	0	0	0	0	0	0.45	0	0.51	0
Grape number		11	12	13	14	15	16	17	18	19	20
	Excellent	0	0	0	0	0	0	1	0	0	0
Red grapes	Good	0.26	1	1	1	1	1	0	0.26	1	1
	Difference	0.74	0	0	0	0	0	0	0.74	0	0
	Excellent	0	0	0.38	1	0.38	0	1	1	0	0.38
White grape	Good	0.38	1	0.62	0	0.62	0.37	0	0	1	0.62
	Difference	0.62	0	0	0	0	0.63	0	0	0	0
Grape number		21	22	23	24	25	26	27	28		
	Excellent	0	0	1	1	0	0	0	——		
Red grapes	Good	1	0.26	0	0	0	1	0.26	——		
	Difference	0	0.74	0	0	1	0	0.74	——		
	Excellent	0	0	0	0	1	0	0	0		
White grape	Good	1	1	0.59	0.38	0	0	0.38	1		
	Difference	0	0	0.41	0.62	0	1	0.62	0		

(2) *Analysis of the Probability that each Grape Falls on Each Level*

Through the calculation results, it can be seen that the probability that the grape variety falls on a certain grade is gradually changed, and one grape may be distributed at most two adjacent grades. This phenomenon reflects the gradual change of the grape quality and the quality of the grape. Not suddenly changing from one level to another.

The reason for this phenomenon is that the grapes are grown in the natural environment, and its various indicators are affected by various factors such as its growth environment and planting management. Therefore, its nature must be gradual, which is reflected in the model. Has a certain degree of instability. At the same time, this also shows that the model is in line with the actual situation.

(3) *The Significance of the Magnitude of the Difference in Each Level*

The greater the difference between the two grades, the greater the probability that the grape is closer to the two levels. The lower the difference in the probability of falling between the two levels, indicating that the grape belongs to the edge of the rank. In extreme love under the circumstance, the probability of falling on a certain two levels is 0.5, which indicates that the quality of this grape is located at the critical point of the two levels.

(4) *Determine the Grade of the Grape based on the Probability of the Determination*

According to the above, when determining the grape grade, select the grade with higher probability, if extreme both levels have a probability of 0.5, and the uniform rule is to choose a lower level. The results of grading each grape sample according to the data in Table 1 are as follows:

According to the results of Table 2, it is found that both the red grape and the white grape have the characteristics of good grades, low grades and poor grades, showing the form of two large heads in the middle, and the quality of the grapes exhibits a normal distribution. This feature of the wine grape grading is consistent with the actual life, indicating that the model is practical.

Table 2. Classification of wine grapes.

	Red grapes	White grape
Excellent grade	1, 2, 3, 9, 10, 17, 23, 24	No. 6, No. 14, No. 17, No. 18, No. 25
Good grade	5, 6, 7, 12, 13, 14, 15, 15, 16, 19, 21, 26	1, 2, 3, 4, 5, 7, 8, 10, 12, 13, 15, 19, 20, 21, 22, 23, 28
Difference level	4, 8, 11, 18, 22, 25, 27	9, 9th, 16th, 24th, 26th, 27th

C. *Classification of Wine Grapes when considering the influence of Aromatic Substances*

(1) Using the Monte Carlo algorithm to calculate the probability of each grape at each level for 100 times, the probability data of each grape can be obtained by analyzing the obtained probability data.

Table 3. Probability of wine grape grading at each level when considering aromatic substances.

Grape number		1	2	3	4	5	6	7	8	9	10
Red grapes	Excellent	0	0.17	0	0	0	0	0	0	1	1
	Good	1	0.83	1	0.18	1	1	1	1	0	0
	Difference	0	0	0	0.82	0	0	0	0	0	0
White grape	Excellent	0	0	0.28	0.32	0	0.51	0	0.04	0	0.5
	Good	1	1	0.72	0.68	1	0.49	1	0.96	1	0.5
	Difference	0	0	0	0	0	0	0	0	0	0

Grape number		11	12	13	14	15	16	17	18	19	20
Red grapes	Excellent	0	0	0	0	0	0	1	0	0	0
	Good	0.18	1	1	1	1	1	0	0.18	1	1
	Difference	0.82	0	0	0	0	0	0	0.82	0	0
White grape	Excellent	0	0	0.51	0	0	0	0.99	1	0	0.51
	Good	0.99	1	0.49	1	1	0.91	0.01	0	1	0.49
	Difference	0.01	0	0	0	0	0.09	0	0	0	0
Grape number		21	22	23	24	25	26	.27	28		
Red grapes	Excellent	0	0	1	1	0	0	0	——		
	Good	1	1	0	0	1	1	1	——		
	Difference	0	0	0	0	0	0	0	——		
White grape	Excellent	0	0	0	0	0.55	0	0	0		
	Good	1	1	1	1	0.45	0.49	1	1		
	Difference	0	0	0	0	0	0.51	0	0		

(2) *Determine the Grade of the Grape Based on the Probability of the Determination*

When the fragrance is considered, the probability of the wine grape grading falling at each level and the probability difference are large. The small meaning is the same as the above, and will not be repeated here. The grape grading under the new model is as follows:

Table 4. Classification of grapes when considering aromatic substances

	Red grapes	White grape
Excellent grade	9, 10, 17, 23, 24	6,13, 17, 18, 20,25
Good grade	1, 2, 3, 5, 6, 7, 8,12, 13,.14,15,16, 18,19, 20, 21, 22, 25, 26, 27	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 14, 15, 16, 19, 21, 22 , 23, 24, 27, 28
Difference level	4, 8, 11,	. 26

Comparing the grading results of aromatic substances with the grading results without considering aromatic substances, it was found that the number of grapes at the superior grade and the poor grade was reduced when considering the aromatic substances, and the grading of the grapes was concentrated to a good grade.

In particular, White Grape No. 13 is a good grade when it does not consider aromatic substances, and it is a good grade when considering aromatic substances; the probability that red grapes 1, 2, and 3 are excellent grades regardless of aromatic substances is 1, considering aromatic When they are substances, they belong to a good grade; red grapes No. 8 and No. 25 have a probability of being a poor grade when considering no aromatic substances, and they are of a good grade when considering aromatic substances; this indicates that the influence of aromatic substances on the quality of grapes is obvious. This is consistent with the previous information and the intuitive feeling of grape quality in life, indicating that it is practical to consider aromatic substances.

Regardless of whether or not the grape's aroma index is considered, the final classification results of the grapes are characterized by “big middle and small”, which reflects the consistency of the two models. This distribution is consistent with the reality of life.

IV. THE CONCLUSION

The model adopted in this paper is based on the clustering center of each index obtained by K-means algorithm, so that it can be concluded that any grape sample is based on its physical and chemical index and wine quality classification, and has strong practicability. In addition, the Monte Carlo algorithm can improve the stability of the model and make the classification of the grapes more reliable. At the same time, it retains certain unstable factors, which reflects the continuous change of the quality of the grapes under natural growth conditions, making the model more consistent. The actual situation. Since the aromatic substances have a certain influence on the quality of the wine, the addition of the aromatic substances on the basis of the original model can more comprehensively classify the wine grapes. However, after adding the indicator of aromatic substances, the amount of data is further increased, and the data relationship is more complicated, which increases the difficulty of solving the model.

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