

Research Article

The Application of Grape Grading Based on PCA and Fuzzy Evaluation

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Abstract: This study grades the wine grape based on the data of physical and chemical indexes of wine grape and the quality of wine in 2012 CUMCM. Since the physical and chemical indexes of wine grape are numerous, we firstly adopt principal component analysis to select the main physical and chemical indexes which can represent most of the property of wine grape. Then, we take the comprehensive score of wine quality as the quality index of wine grape. Later, taking the contribution rate in principal component analysis and quality of wine as the fuzzy evaluation weights, we set up a fuzzy comprehensive evaluation model for the grading of wine grape according to the international standard of wine grade. The grades of the red and white wine grape all belong to 3, 4 and 5 grade, respectively and the grading result can well prove that the quality of wine can reflect the quality of wine grape to some extent.

Keywords: PCA fuzzy evaluation, wine grape grading

INTRODUCTION

The quality of wine grape has direct influence on the quality of wine. The Physical and Chemical Indexes (PCIs) of wine grape can also reflect the quality of grape. Thus, the PCIs of wine grape and the quality index of wine can be taken as one criteria for the grading of wine grape. In fact, there are more than 30 usual first-grade PCIs of wine grape. The purpose of this study is grading the grape according to the data of PCIs of wine and grape, as well as the data of comprehensive wine evaluation given by the wine tasters.

Luo (2001) analyzed fuzzy mathematics were applied to sensory evaluation in the determination of juice drink and deduced the relationship between the Kiwi fruit juice drinks and their formula.

Huo (2004) also used fuzzy mathematics in evaluating the food sensual quality to make fuzzy effective control of wine quality inspection and product quality.

Wang and Feng (2011) applied Fuzzy Synthetic Evaluation in the sense estimation of Dry Red Wine. They unified 5 influence factors, including the appearance, the fragrance, the taste, the typical nature, the synthesis quality as the coordinative index of discourse domain on wine and classified 5 ranks. The results of the fuzzy synthetic evaluation about coordination were analyzed by vector analysis.

Specially, Xiao *et al.* (2011) studied the wine production process; their best formulation of the fermentation liquor is determined by orthogonal test design and the method of fuzzy mathematics

evaluation. The best formula is that wine 150 g, sucrose 24 g, Angel yeast 0.65 g.

However, they did not analyze the physical and chemical indexes of the formula. In addition, more than 70 kinds of aromatic substances exist in wine grape and different substances have complicated relationship with each other. Therefore, to extract the indexes that can mostly reflect the quality of wine grape is a must. At present, the hedonic scoring system held by the senior wine tasters is the main method applied for wine evaluation. Data study is based on the results of comprehensive wine evaluation given by the wine tasters of Group B presented in 2012 CUMCM. Hence, this study just combines the traditional hedonic scores of wine with the major PCIs of wine grape to deal with the grading of the grape quality.

We analyzed the PCIs and classified them into first-class index and second-class index. Furthermore, we removed the abnormal data and graded the wine grapes and aromatic substances in wine.

As for the model, PCA (Principal Component Analysis) was utilized to analyzed PCIs of wine grape. Finally, we built the Fuzzy Comprehensive Evaluation Model for the Grading of Grape. And the grading result can well prove that the quality of wine can reflect the quality of wine grape to some extent.

MATERIALS AND METHODS

Materials: This study grades wine grape into different grades according to the PCIs of the wine grape and the quality of wine.

Data in 2012 CUMCM presents many PCIs of wine grape (including 30 first-grade indexes and 73 kinds of aromatic substances), so if we take all these PCIs of wine grape into consideration, the calculation will be too complicated. Besides, there are large correlations between some PCIs, which will be repeated when we study the PCIs of wine grape, affecting the analysis result.

By further analysis, we find that PCIs can be divided into the first-grade index and the second-grade index, among which the second-grade index is the subdivision of the first-grade index. Since there are 73 kinds of aromatic substances in wine grape, based on their chemical structure, this study gradeify the aromatic substances in the wine grape into six categories: alcohol compounds, ester compounds, organic acid compounds, carbonyl compounds, terpene compounds and sulphur compounds. For aromatic substances which not belong to these six categories, they are gradeified into another category (Lei *et al.*, 2008). The amounts of various kinds of substances in every kind of wine grape sample are also calculated study.

Methods: In order to take the PCIs of wine grape into full consideration, this study apply PCA to analyze the PCIs of wine grape on the premise of gradeifying the aromatic substances of wine grape based on their chemical structure. Then, we get most of the PCIs of winegrape's physicochemical properties. Based on that, this study make an analysis of the effect of wine grape's PCI son the grading of wine grape according to the PICs which can reflect the major properties of wine grape.

In addition, we still need to take wine quality into consideration, whose index can be get by calculating

the mean value of the comprehensive scores of every wine sample.

Thus, take the second-grade PCIs of wine grape, categorized aromatic substances and the quality index of wine as a factor set, we set up a fuzzy comprehensive evaluation model to gradeify the wine grape.

DATA PREPROCESSING

Removal of the abnormal data: By detailed analysis, we can find some data are abnormal, which are usually much larger than other data. For example, the measured value of a hundred white wine grapes at the third time is 2226.1, which is much larger than that of the first time and second time. This may result from the faults in data recording and other factors. Therefore, we should adjust these data.

Equalization of the multi-measuring data: Several PCIs are multi-measured, so we take the average values as the values of their PCIs.

Grading of wine grapes and aromatic substances in wine: Since there are numerous kinds of wine grapes and aromatic substances in wine, according to the chemical structure of aromatic substances, this study divided these data into six categories: alcohol compounds, ester compounds, organic acid compounds, carbonyl compounds, terpene compounds and sulphur compounds. For aromatic substances which not belong to these six categories, they are gradeified into another category. The specific criteria for the grading of aromatic substances in red wine are listed in Table 1.

Seeing from Table 1, we can find that the aromatic substances in red wine are divided into 10 categories

Table 1: Specific criteria for the grading of aromatic substances in red wine

Ester	Ethyl acetate	Ethyl propionate	Hexadecanoic acid, ethyl ester
	Ethyl butyrate	Ethyl caprylate	Acetic acid, 2-phenylethyl ester
	Amyl acetate	Ethyl caproate	Octanoic acid, 3-methylbutyl ester
	Ethyl oenanthate	Ethyl lactate	2-hexenoic acid, ethyl ester
	Heptyl acetate	Methyl caprylate	Acetic acid, 2-methylpropyl ester
	Isoamyl caproate	Octyl acetate	Butanedioic acid, diethyl ester
	Ethyl pelargonate	Methyl caprate	Pentadecanoic acid, 3-methylbutyl ester
	Hexyl acetate	Propyl caprylate	Ethyl trans-4-decenoate
	Ethyl laurate	Ethyl caprate	Tetradecanoic acid, ethyl ester
	n-propyl acetate	Glycerol	1, 2-benzenedicarboxylic acid, bis (2-methylpropyl) ester
	1-butanol, 3-methyl-, acetate		
Alcohol	1-heptanol	1-propanol, 2-phenoxy-	1, 4-benzenediol, 2, 5-bis (1, 1-dimethylethyl)-
	1-propyl alcohol	1-Propanol, 2-methyl-	6-octen-1-ol, 3, 7-dimethyl-, (R)-
	1- hexanol	Isosorbide	2-ethyl-1-hexanol
	2- nonanol	Benzyl alcohol	1, 6-octadien-3-ol, 3, 7-dimethyl-
	1-EH	Phenylethyl alcohol	1, 5, 7-octatrien-3-ol, 3, 7-dimethyl-
	Alconol	1- butanol, 3-methyl-	1-propanol, 3- (methylthio)-
Acid	Acetic acid	Ethyl hydrogen succinate	2-methyl propyl
	Benzoic acid	Dodecanoic acid	Butyric acid
	Caprylic acid	2-decanoic acid	
Ketone	2, 3-pentanedione	2-pyrrolidinone	2-octanone
Alkene	Limonene	Styrene	
Ether	Ethyl geranyl ether	Diethylene glycol monoethyl ether	
Alkane	n-tridecane	n-undecane	
	7-methoxy-2, 2, 4, 8-tetramethyltricyclo [5.3.1.0 (4, 11)] undecane		
Phenol	Phenol, 2, 4-bis (1, 1-dimethylethyl)-	2-Methoxy-4-vinylphenol	
Biphenyl	1, 1'-biphenyl, 4-methyl-		
Furan	Benzofuran, 2, 3-dihydro-		

Table 2: The grading of aromatic substances in red wine

Wine No. of	Ester	Alcohol	Acid	Ketone	Alkene	Ether	Alkane	Phenol	Aldehyde	4- methyl -1,1'- biphenyl	2, 3-dihydrobenz of uran
1	308.65	130.91	19.91	7.74	2.14	1.22	3.72	0.92	2.22	0.92	2.45
2	223.43	174.31	10.71	4.94	4.12	8.13	0.51	0.00	2.41	-	0.77
3	121.30	185.93	5.22	1.22	1.23	1.83	0.51	0.00	2.64	-	-
4	242.76	108.98	13.61	3.26	3.48	1.40	2.36	2.39	1.72	-	-
5	266.13	124.29	12.74	3.37	6.88	4.03	2.66	1.72	1.92	-	-
6	209.68	193.76	6.35	4.24	4.32	6.19	0.31	32.42	4.14	-	-
7	198.40	100.75	9.92	3.55	4.45	3.56	0.72	42.69	1.40	-	-
8	146.04	163.49	9.31	2.95	1.27	0.09	0.34	0.00	3.45	-	0.18
9	201.80	136.38	9.90	3.36	4.10	1.80	1.10	0.59	2.09	-	-
10	186.02	94.87	10.89	3.68	2.31	0.04	1.09	0.31	1.74	-	-
11	105.59	89.49	12.08	2.59	0.10	1.08	0.65	1.16	1.34	0.10	2.12
12	222.52	171.68	10.92	2.74	0.22	2.94	0.28	0.00	2.46	-	1.94
13	218.34	121.32	13.57	3.18	2.69	1.79	0.86	26.26	1.58	-	-
14	117.45	57.56	8.80	2.10	0.00	1.30	0.81	0.34	0.64	0.17	0.52
15	258.96	137.73	11.49	4.77	4.43	9.93	0.51	0.00	1.44	-	0.52
16	238.35	98.68	10.55	3.70	4.33	3.39	1.38	0.20	4.47	-	-
17	280.84	148.97	11.80	3.45	6.61	10.37	0.44	0.00	2.19	-	0.30
18	75.81	202.54	9.17	2.67	0.15	4.28	0.51	0.00	4.60	-	-
19	221.74	126.30	12.00	3.78	3.17	1.95	1.75	0.63	1.99	-	-
20	127.78	143.43	7.19	2.62	1.54	3.62	0.41	0.42	1.74	-	-
21	182.38	143.99	8.00	3.90	6.85	1.99	0.52	1.90	2.18	-	-
22	376.90	137.65	13.24	4.02	8.60	1.69	3.49	0.78	2.00	-	0.39
23	238.58	137.48	15.03	4.59	6.23	9.39	2.61	0.00	1.78	-	-
24	256.92	152.97	13.11	4.26	3.59	7.79	0.51	0.51	5.43	-	0.51
25	186.40	87.04	19.32	3.59	2.33	2.45	0.99	29.34	1.40	-	0.47
26	223.21	97.87	12.80	3.68	2.48	1.00	1.40	0.76	2.62	-	-
27	277.89	136.00	8.90	3.73	3.04	2.80	0.42	87.63	1.57	-	-

Table 3: Main indexes of red grape after PCA

Major indexes of red grape	Contribution rate	Contribution rate ranking	Major indexes of white grape	Contribution rate	Contribution rate ranking
Total amino acid	0.111	1	Total amino acid	0.128	1
Protein	0.101	2	Protein	0.114	2
Content of VC	0.069	3	Content of VC	0.078	3
Anthocyanin	0.064	4	Anthocyanin	0.074	4
Tartratic acid	0.061	5	Tartratic acid	0.071	5
Malic acid	0.055	6	Malic acid	0.064	6
Citric acid	0.049	7	Citric acid	0.056	7
PPO activity	0.046	8	PPO activity	0.052	8
Browning degree	0.044	9	Browning degree	0.049	9
Tannin	0.038	10	DPPH free radical	0.044	10
Resveratrol	0.036	11	Total phenol	0.039	11
Total flavonoids of grape	0.035	12	Tannin	0.035	12
Flavonol	0.034	13	Total flavonoids of grape	0.032	13
Total sugar	0.032	14	Resveratrol	0.031	14
Reducing sugar	0.031	15	Cumulative contribution rate	0.867	-
Quality of cluster	0.027	16			
The proportion of stem	0.024	17			
Cumulative contribution rate	0.856	-			

Table 4: The evaluation result of the red wine quality

No. of the red wine sample	Evaluation result	No. of the red wine sample	Evaluation result
1	67.98	15	66.13
2	73.58	16	65.97
3	73.95	17	74.50
4	71.12	18	63.60
5	72.35	19	72.21
6	65.91	20	74.21
7	64.70	21	71.47
8	65.17	22	70.43
9	78.04	23	76.74
10	68.61	24	71.60
11	61.66	25	67.05
12	68.53	26	72.22
13	69.37	27	71.20
14	72.41		

basing on the their chemical structure, which can not only greatly benefit the disposal of the aromatic substance in the later model, but also fully make use of the data available.

Based on the criteria in Table 1, we use Excel to process the data to get the grading of aromatic substances in red wine, which is presented in Table 2.

Symbol “-” in Table 2 represents that this substance does not exist in this wine and it has the same

meaning in the Table 3 and 4. From Table 2, we can find that aromatic substances in red wine are divided into 11 categories and the first nine 9 categories are the major categories. We adopt similar methods to gradeify the aromatic substances in wine grape.

RESULTS AND DISCUSSION

The PCA for the PCIs of wine grape: This study gradeify the wine grape according to the PCIs of wine grape and the quality of wine. Since the aromatic substances in wine grape are numerous, overlapping effect may exist. Thus, we make grading of the aromatic substances based on the chemical structure and take alcohol and ester as the first-grade index to get overall PCIs of the wine grape.

After the first-grade index combined with aromatic substance there are still 41 PCIs in wine grape. On one hand, multi-index can fully reflect the propertys of wine grape; on the other hand, it also leads to the complexity of analysis. Correlation may exist among the PCIs of wine grape, which can leads to the overlapping of

information. In order to overcome the correlation and overlapping, PCA is adopted for dimension reduction. We can get the PCIs which can mostly represent the physicochemical property of wine grape with little loss of the information. Moreover, basically there is no correlation among the PCIs selected.

By using MATLAB, we can obtain that there are 17 main PCIs, which can affect the grading of red grape and 14 main PCIs, which can affect the grading of white grape grading. The result is shown as Table 3.

From Table 3, we can find that these 17 PCIs in red grape can represent nearly 85.6% of its property and 14 PCIs in white grape can represent nearly 86.7% of its property. Besides, the principle components of the red grape and white grape don't include aromatic substance, which means aromatic substances have little effect on the overall property and grading of the red grape and white grape.

Dealing with the effect of wine quality on the grading of grape: The study above shows that the evaluation result of the sensory quality of wine given by the wine tasters in Group B is more reliable. Thus, the quality index of wine can be expressed by the average comprehensive score of the scores given by wine tasters in Group B, which are processed by the confidence interval. The evaluation result of the red wine quality are presented in Table 4.

From Table 4, we can conclude that there is small difference among the quality of the 27 kinds of red wine samples given by the sensory evaluation of the wine tasters and the evaluation scores ranging from 60 to 79. In fact, the quality of the wine sample greatly reflect the grade of the grape. Hence, the grape quality determined by the quality of wine also differs slightly, which provides the referring grade for the grading of grape.

The fuzzy comprehensive evaluation model for the grading of grape: By analysis, we can find that the quality of wine grape has direct influence on the quality of wine. Similarly, quality of wine can reflect the quality of wine grape to some extent. Thus, this study takes the evaluation result of wine given by the wine tasters in Group B as the overall sensory index for the wine grape. Combined this with PCIs of grape in PCA, we set up the grape fuzzy comprehensive evaluation model for the grading of grape.

Determining the field of factors of wine grape: $U = (u_1, u_2, \dots, u_m, S_kR)$, among which u_1, u_2, \dots, u_m represents the m principle component indexes of wine grape.

Determining the grade set: According to the latest national standard GBT 15038-2006 for wine (National Standard of the People's Republic of China GB/T 15038, 2006) the grape study can be divided into five grades {first grade, second grade, third grade, fourth

Table 5: The weight distribution of wine grape

Field of factors	Contribution rate	Weight
Total amino acid	0.1108	0.05540
Protein	0.1009	0.05045
VC content of	0.0688	0.03440
Anthocyanin	0.0635	0.03175
Tartratic acid	0.0608	0.03040
Malic acid	0.0549	0.02745
Citric acid	0.0494	0.02470
PPO activity	0.0456	0.02280
Browning degree	0.0439	0.02195
Tannin	0.0381	0.01905
Resveratrol	0.0356	0.01780
Total flavonoids of grape	0.0350	0.01750
Flavonol	0.0336	0.01680
Total sugar	0.0322	0.01610
Reducing sugar	0.0313	0.01565
Quality of cluster	0.0273	0.01365
The proportion of stem	0.0242	0.01210
Evaluation result of red wine	0.5000	0.50000

Table 6: Results of the grading of wine grape

Grade of red grape	No. of red wine grape
3 grade	1, 2, 3, 8, 9, 14, 21, 23
4 grade	17, 5, 19, 24
5 grade	4, 6, 7, 10, 11, 12, 13, 15, 16, 18, 20, 22, 25, 26, 27
Grade of white grape	No. of white wine grape
3 grade	1, 3, 5, 9, 10, 15, 17, 20, 21, 22, 24, 27, 28
4 grade	4, 6, 7, 8, 13, 14, 18, 19, 23, 25
5 grade	2, 11, 12, 16, 26

grade, fifth grade}, where the first grade is the highest grade and the fifth grade is the lowest grade and their corresponding scores are:

$$V = \begin{cases} 0.9 - 1.00, \text{ first grade} \\ 0.8 - 0.90, \text{ second grade} \\ 0.7 - 0.79, \text{ third grade} \\ 0.65 - 0.69, \text{ fourth grade} \\ \leq 0.65, \text{ fifth grade} \end{cases}$$

Determining the weight of evaluation factors: Since the quality of wine can greatly reflect the quality of the wine grape, so the PCIs of wine grape and the wine quality are of the same importance to the grading of wine grape. That means the first-grade weight ratio between the principle component indexes of wine grape and that of the wine quality is 0.5:0.5. Among the principle component indexes of wine grape, different indexes corresponds to different contribution rates, which equals to second-grade weight. Thus, the comprehensive weight of different principle component indexes can be expressed as the product of the first-grade weight and the second-grade weight. The result is shown as Table 5.

Standardize the weight we get and take them down as $E = (e_1, e_2, \dots, e_{m+1})$, in which m represents the m principle component indexes of grape and e_{m+1} represents the weight of wine evaluation result.

Solution of the fuzzy comprehensive evaluation model for the grading of grape: By adopting the MATLAB, we can get the solution result of the model as shown in Table 6.

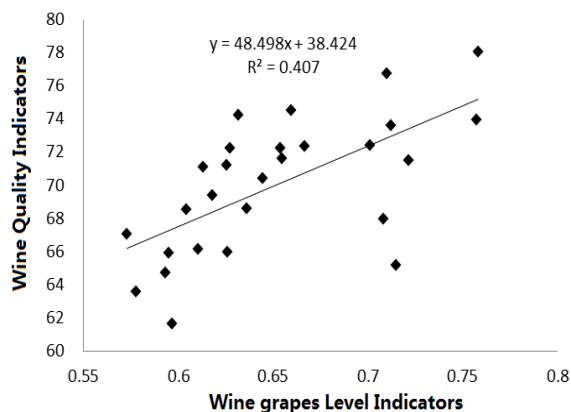


Fig. 1: The fitting analysis of quality index of red wine and grading indexes of red wine grape

Table 7: The grading result by selecting the first 20 samples of red wine grape

Grade of red grape	No. of the red wine grape
3 grade	1, 2, 3, 5, 8, 9, 14
4 grade	16, 17, 19
5 grade	4, 6, 7, 10, 15, 11, 12, 13, 16, 18, 20

From Table 6, we can see that based on the grading criteria, all the wine grapes belong to the third to fifth grade. And according to the latest national standard GB/T 15038-2006 for wine, the grading of wine grape is consistent with the grade of corresponding wine quality.

CONCLUSION

Analysis of the stability and reliability of the model:

In order to examine the relationship between the wine quality and the grade of wine grape and further verify the reliability of model, this study fits the final average comprehensive score of the sensory quality of wine and the grade of the wine grape. By analyzing the result of fitting, we make an analysis of the model's reliability. Firstly, take the quality of red wine and the grade of red wine grape as an example to fit the data. Then, take the average comprehensive score of the scores given by wine tasters in Group B, which are processed by the confidence interval as the quality index of red wine. For the quality factor of the red wine grape, we use the grading criteria of red wine grape as an example. The fitting result is shown as Table 1.

From Fig. 1, we can find that large interaction exist between the grading indexes of red wine grape and the quality index of red wine, the result of linear fitting is

just ordinary and R^2 is 0.407. That means the grading indexes of red wine grape can partly determine the quality index of the responding red wine, namely the result of the model is of certain reliability. Besides, it also means the reliability of model is still need to be strengthened. Take numerous factors into consideration, this result is quite good.

Sensitivity analysis: Sensitivity analysis means to check when variables of the model change, how the result will vary. During the process of analyzing and modeling, this study select relevant data of all wine grape and wine. To make a sensitivity analysis of the model, we reduce the samples adopted, namely substituting the data available to into the model to test whether the result of the model will obviously change.

Combining PCIs of wine grape with the quality of wine, this study adopts fuzzy comprehensive evaluation method to classify wine grape. In order to make a sensitivity analysis of the model, we just select the first 20 samples of red wine grape and adopt the same method. The grading result of red wine grape can be seen in Table 7.

Table 7, this study makes an comparison between the result of just selecting the first 20 sample and the original result (in Table 6) and finds that their results are basically the same and only the grades of red wine grape of No. 5 and 16 change.

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