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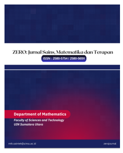

The Impact of Using A Linear Model for the Ordinal Response of Mixture Experiments

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ABSTRACT

In a sensory test, the response is a Likert scale, which belongs to the ordinal scale. The ordinal response can be analyzed using a linear model approach; however, this approach can be misleading. This research aims to compare three different methods for ordinal response: the average score, the second-order Scheffe model, and the ordinal logistic model. The case study focused on the response to the taste of cookies resulting from the mixture experiment. The mixture experiment is one type of experimental design which is commonly used for product formulation. The research involved three ingredients with different lower bonds. The D-optimal design which also the {3,2} simplex-lattice design was chosen for the experiment. The three methods were conducted, and they all yielded the same results for the optimum composition; however, the ordinal model provided more information about the data's characteristics. The optimal formulation of each ingredient was 10%, 20%, 70%.

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1. INTRODUCTION

In order to evaluate taste in the food industry, the researchers use the sensory test. The sensory test response is the Likert scale that belongs to the ordinal scale [1]. The scale in which categorical and ordered from low to high is called an ordinal scale [2]. In the context of regression, a model is defined based on the measurement scale of a response variable. The linear model is a model when the response variable is numeric and follows a normal distribution. However, suppose the response variable is categorical. In that case, the analysis using a linear model will not appropriate because the model will have worse goodness of fits, and the model is not accurate in prediction. In this case, nonlinear models are used [3]. Logistic regression belongs to a nonlinear model because the distribution assumption is a binomial distribution. [4] discussed how to use logistic regression instead of linear regression when the response is dichotomous. Furthermore, [5] discussed the ordinal regression in which the response is an ordinal scale. [6] also gave inside detail about the violation of the standard model in ordinal regression developed by [5].

In recent years, [7] discussed the advantage of ordinal logistic regression to analyze the sensory data that used a seven-point intensity scale. The researchers used the mixture experiment to formulate the formula. The seven-point intensity scale is treated as an interval scale when the Scheffé model is assumed. However, this approach brought evil goodness of fit. Hence, The paper contrasted the proportional odd and the stereotype model. Both models belong to ordinal logistic models. The mixture experiment's unique feature is multi-collinearity among the model's factors because of the two main constraints of mixture experiments. The results show that the odd proportional model failed to achieve the appropriate interpretation; meanwhile, the stereotype model reached better interpretation when the categories are smaller.

In this paper, the authors used an optimal design approach to generate the design. Optimal design is a branch of experimental design seeking an optimal design based on a particular optimality criterion [8]. [9] addressed detail about various optimality criteria such as D-optimality criterion and V- or I-optimality criterion. The D-optimality criterion is a criterion that focuses on precision on parameter and widely used in an application; meanwhile, the I-optimality criterion is a criterion that focuses on precision on average prediction variance entire the experimental region.

In context response surface methodology, [10], and [11] denoted that I-optimal designs usually perform well in terms of D-optimality criterion but not vice versa. [12], [13] [14] and [15] addressed the D-optimality criterion in their research. However, [16] It has been mentioned that the mixture experiment is a special case for response surface methodology. Mixture experiments belong to response surface methodology because the levels of factors are quantitative proportions. Hence, this paper's reason is considered the optimal design based on the D—and I-optimality criterion.

2. RESEARCH METHOD

The case study involved three ingredients with a specific restriction on proportion. Ingredient 1 and ingredient 2 were at least 10%; respectively, ingredient 3 was at least 60%. The constraints affected the experimental region. Hence, the experimental region is a subset of the whole simplex because of the constraints on proportions. Figure 1 shows the experimental region of the case is a simplex.

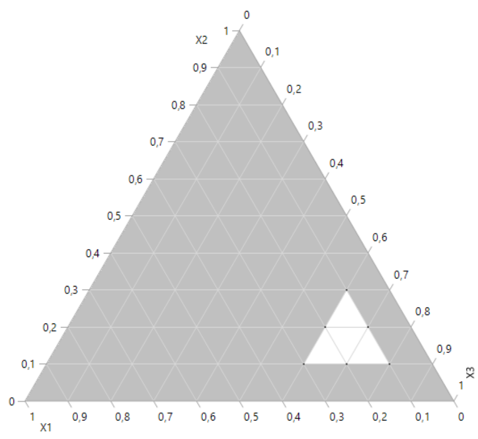


Figure 1. The white area is the experimental region of the case study

2.1 The steps of methodology on this paper are

Generating the simplex mixture design.

The experimental of the D-optimal design and the I-optimal design was twelve. As there are lower bounds on proportions, the experimental region is simplex (Figure 1). The components are transposed into the pseudo components to fit the model, so the new components lie between 0 and 1.

The D-optimal design is searching for a design based on the determinant of the information matrix [17]. Suppose there are q ingredients and x_1, x_2, ..., x_q represents each ingredient's proportion. The second-order Scheffé model is

$$E(Y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \beta_{ij} x_i x_j \tag{1}$$

where Y in Equation (2) represents the response variable, the coefficients β_i represent the pure component's expected response. The pure component is when the proportion of the i-th ingredient equals one. The parameters β_{ij} represent the nonlinear blending properties of binary blending between the i-th ingredient and the jth ingredient. Binary blending is meaning that 50% of the i-th ingredient and 50% of the jth ingredient.

In matrix notation, suppose X is a n x p model matrix with n is the number of experimental runs, and p is the number of the model's parameter. Define matrix M is X'X and the D-optimality criterion is determinant of matrix M, denoted as det(M). To evaluate the design in terms of the D-optimality criterion is using D-efficiency. Formula of the D-efficiency is $(\det(M1)/\det(M2))^{1/p}$. M1 and M2 are the information matrix of Design 1 and Design 2, respectively. If D-efficiency is larger than 1, meaning that Design 1 outperforms than Design 2.

On the contrary, the I-optimal design seeks a design based on minimizing the average prediction variance over the experimental region [17], [18]. The formula of I-optimality criterion is

$$I - optimality\ criterion = \frac{\int_{\chi} \boldsymbol{f^{`}(x) M^{-1} f(x) dx}}{\int_{\chi} \boldsymbol{dx}} \tag{2}$$

In order to evaluate the design based on the average prediction variance is using I-efficiency. The I-efficiency formula is P2/P1, which P1 is the average prediction variance of Design 1; meanwhile, P2 is the average prediction variance of Design 2. Design 1 is better than Design 2 if I-efficiency is larger than 1. To generate both D-optimal design and I-optimal design were applying a coordinate exchange algorithm provided by software JMP.

Furthermore, to compare the optimal designs, to make a visual comparison is utilizing a Fraction of Design Space (FDS). The FDS plot describes the prediction variance, which shows the cumulative distribution of the prediction variance across the entire experimental region. The FDS plot shows more information, such as minimum, average, median, and maximum prediction variance. A good design should have small prediction variances in most areas of the experimental region. The best design by D-efficiency, I-efficiency, and FDS was implemented in the laboratory and conducted the sensory test. Each design point had one replication.

The sensory test was involved ten people of each design point.

In this research was applying the interval scale between 1 and 6. Three different analyses: the average score, the second-order Scheffé model, and the ordinal logistic model were comparing. The ordinal logistic model is a regression analysis in which the response is an ordinal scale. The full model or the odd proportional model of ordinal data for mixture experiment [7] is

$$\text{logit}\ \mathrm{P(Y \leq j)} = \log \frac{\mathrm{P(Y \leq j)}}{\mathrm{P(Y >} j)} = \alpha_j + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 \\ j = 1,2,\ldots,J-1 \tag{3}$$

The big issue in the mixture experiment is multi-collinearity among the ingredient proportions since $x_1 + x_2 + x_3 = 1$. To avoid the multi-collinearity, in this paper, the authors removed x3 from the model since the ingredient 3 had a large proportion in the model, so the reduced model becomes

$$\text{logit}\ \mathrm{P(Y \leq j)} = \log \frac{\mathrm{P(Y \leq j)}}{\mathrm{P(Y >} j)} = \alpha_j + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 \\ j = 1,2,\ldots,J-1 \tag{4}$$

The other analysis results would be compared based on the coefficients model's significance, the optimum composition, and the response prediction.

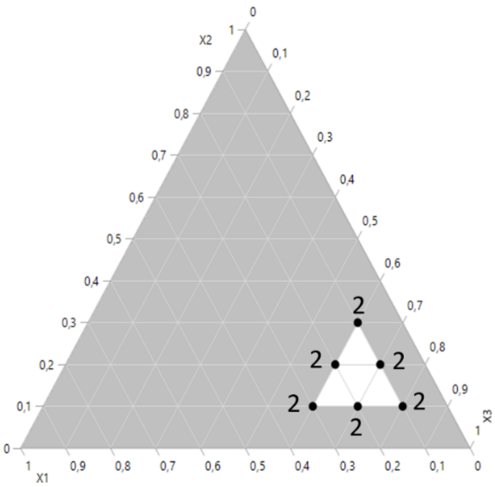
3. RESULT AND ANALYSIS

3.1 The construction of the design

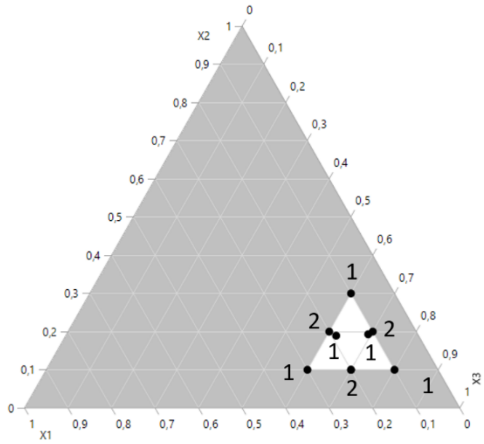
There were three designs for the case study based on the second-order Scheffé model. Figure 1 shows that the experimental region is a simplex, so the mixture design was a {3,2} simplex-lattice design. The mixture design involved six design points with two replication on each. This design is the same as with the D-optimal design (Figure 2(a)). This means that the {3,2} simplex-lattice design was also the D-optimal design. Unlike the D-optimal design, t5%he I-optimal design consisted of eight different design points. Six design points were similar to the D-optimal design; meanwhile, the two other design points closed to the edge points (Figure 2(b)). The design point that lay on the middle of edges had more replicates than the corner design points.

The D-optimality criterion of the D-optimality design was 1,024E-13; meanwhile, the D-optimality criterion of the I-optimality design was 3,614E-14. The D-efficiency of the I-optimal design compared to the D-optimal design was 0.841. It means that the D-optimal design outperformed the I-optimal design in terms of parameter estimation. In contrast, the I-optimal design was better than the D-optimal design in terms of prediction variance. The I-efficiency of the I-optimal design compared to the D-optimal design was 1.143. The FDS plot, as shown in Figure 3, also shows almost 90% of the design space, the prediction variances of the I-optimal design below the ones of the D-optimal design. If Figure (2b) becomes Figure (2c), the I-optimality criterion is quite the same. D-efficiency and I-efficiency of the modified I-optimal design compared to the I-optimal design were 1.030 and 0.989, respectively. Hence, both I-optimal designs had the same performance in terms of prediction variance.

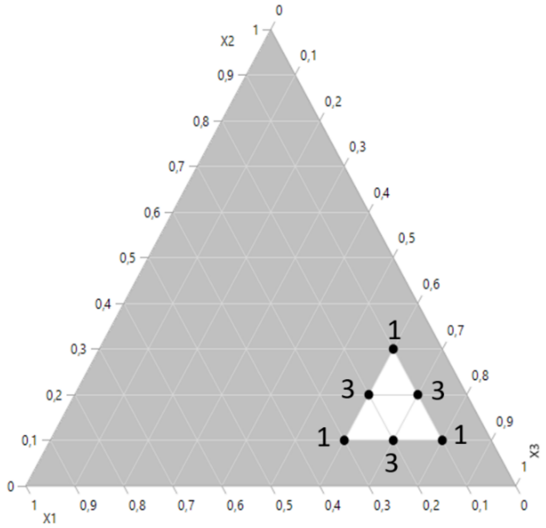
Although the I-optimal designs were better than the D-optimal design in terms of prediction variance, the authors chose the experiment's D-optimal design. The reason was that the D-optimal design had the same replications on each design point, and also, the D-optimal design was similar to the {3,2} simplex-lattice design. In addition, [19] gave overview that D-optimal design outperforms compared to the I-optimal design.



(a) The {3,2} simplex-lattice design and the D optimal design



(b) The I-optimal design



(c) The modified I-optimal design

Figure 2. The {3,2} simplex-lattice design, the D-optimal design, and the I-optimal design of the second-order Scheffé model.

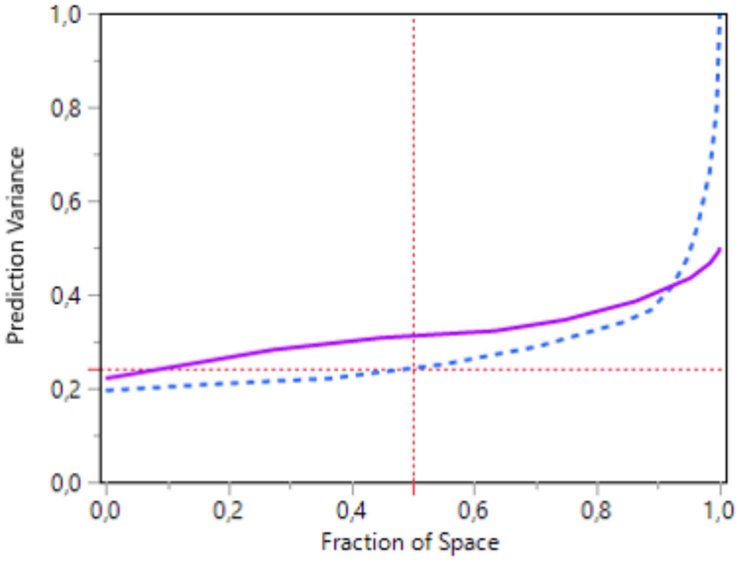


Figure 3. The FDS plot of the I-optimal ( ) and the D-optimal design ( )

3.2 The analysis of the data

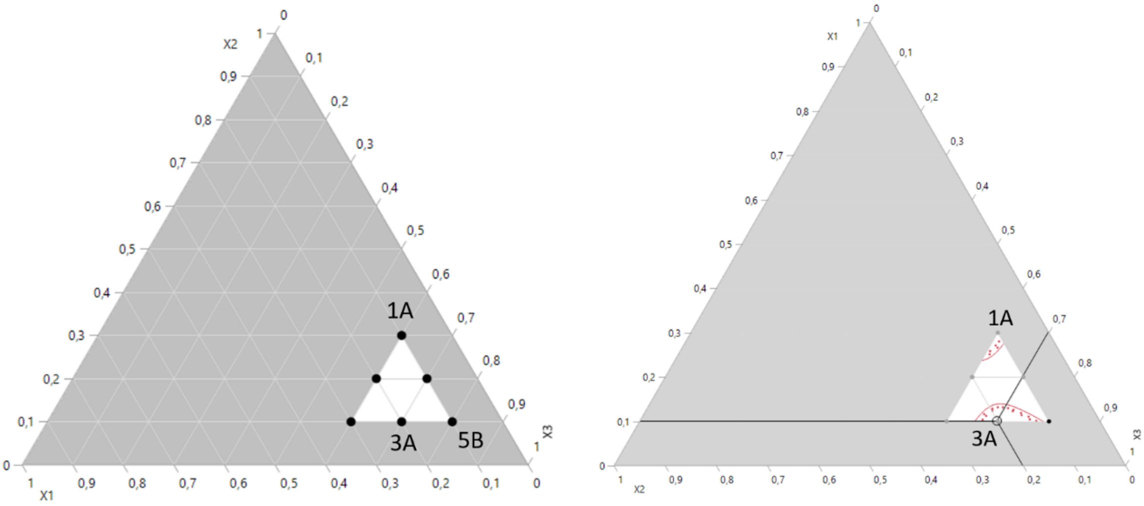
Table 1 shows the 12 design points of the D-optimal design, with each design point weighing 200 grams. Table 1 involves the composition of each design point in percentage and grams. Label "A" refers to the first replication. Meanwhile, label "B" refers to the second replication. Three analyses would be compared to determine the consistency of results or the best method to choose corresponding to the response's ordinal scale.

The average score method

Table 1 also shows the average score of the sensory test of each design point. Based on the average score, the first rank was the composition with 60% of ingredient 1, 30% of ingredient 2, and 10% of ingredient 3 (label "1A"). Two design points had the same average score. The compositions of the first design point were 10% of ingredient 1, 20% of ingredient 2, 70% of ingredient 3 (label "3A") meanwhile the compositions of the second design point was 10% of ingredient 1 and 2, respectively, and 80% of ingredient 3 (label "5B"). Label "1A" and label "5B" lay on the corner, and label "3A" lay on the middle of the edge. Figure 4(a) shows the position of the design points.

Table 1. The 12 design points of the D-optimal design and the results of the sensory test

Run	x1(%)	x2(%)	x3(%)	x1(gr)	x2(gr)	x3(gr)	Average score
1A	30	10	60	60	20	120	4.80
2A	20	20	60	40	40	120	4.20
3A	10	20	70	20	40	140	4.60
4A	10	30	60	20	60	120	3.73
5A	10	10	80	20	20	160	3.82
6A	20	10	70	40	20	140	3.73
1B	30	10	60	60	20	120	4.27
2B	20	20	60	40	40	120	4.09
3B	10	20	70	20	40	140	4.45
4B	10	30	60	20	60	120	3.70
5B	10	10	80	20	20	160	4.60
6B	20	10	70	40	20	140	4.10



(a) The average score (b) The mixture model

Figure 4. The optimum condition of the average score and the second-degree Scheffé model

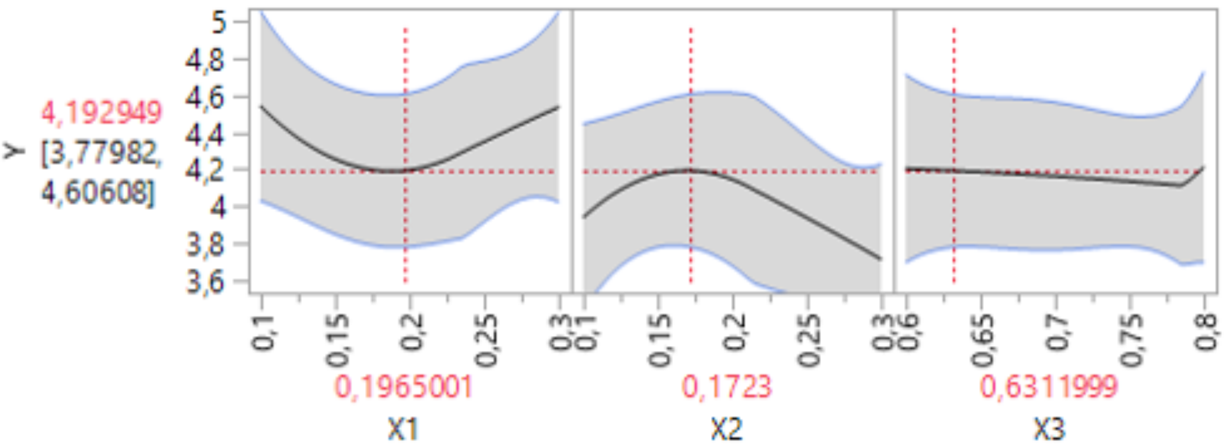


Figure 5. Profiling plot of the second-degree Scheffé model

The second-order Scheffé model

Further analysis is analyzing the data with the second-order Scheffé model. The response was the average score. Table 3 shows the estimation of the parameter model. The bad news was that no coefficients were significant at $\alpha = 5\%$, but some terms were significant at $\alpha = 10\%$. Table 3 shows the estimation of the parameter model which some terms were significant at $\alpha = 10\%$. The model's coefficient determination was 67%, meaning that the model explained the variability of the average score of around 67%. [20] also did a research about the Likert scale in mixture experimet and had the same inside. In detail, Figure 4 shows the profiling plot of the model. Ingredients 1 and 2 had a quadratic effect, whereas ingredient 3 had a linear effect, and Figure 3 shows the optimum condition based on the model. The optimum condition achieved when the compositions were (10%, 20%, 70%) and (30%, 10%, 60%) of each ingredient. The first composition was the design point with the label "3A," and the second one was the design point with the label "1A". Those two compositions also appeared at the average score method. Figure 4b shows the position of both compositions.

Table 3. Coefficient estimation of second-degree Scheffé model

Components	Coefficients	Std. error	t-hit	p-value
x1(Mixture)	0,338	0,145	2,330	0,059
x2(Mixture)	-0,314	0,145	-2,170	0,073
x3(Mixture)	0,038	0,018	2,200	0,070
x1*x2	0,000	0,003	0,080	0,941
x1*x3	-0,005	0,003	-1,780	0,126
x2*x3	0,006	0,003	2,180	0,072

The ordinal logistic model

Table 4. Coefficient estimation of the reduced ordinal logistic model

Term	Estimates	Std. error	Chisquare	Prob > Chisq
Intercept[1]	-7,128	3,472	4,210	0,040*
Intercept[2]	-6,545	3,457	3,590	0,058
Intercept[3]	-4,861	3,436	2,000	0,157
Intercept[4]	-2,848	3,415	0,700	0,404
Intercept[5]	-0,234	3,427	0,000	0,946
X1(Mixture)	-59,633	26,569	5,040	0,025*
X2(Mixture)	36,807	26,211	1,970	0,160
X1*X2	-4,891	49,573	0,010	0,921
X1*X3	107,736	50,372	4,570	0,033*
X2*X3	-38,664	49,604	0,610	0,436

*Significant at α = 5%

Table 4 shows the estimation of parameters of the reduced ordinal logistic model. The categorical reference of the response was score 6. The estimate of the intercept for scores 1 to 5 was negative, indicating that respondents were more likely to choose score 6 for the cookies. Furthermore, the term x_1 and $x_1{}^*x_3$ are significant. These results show that the probability that the score is higher is related to ingredient 1. In addition, the probability of the score does not only depend on the ingredient 1, but also depends on the ingredient 3. This result is expected to be substantial since the profiling plot shows that the first ingredient should be considerable. The composition of 30% of ingredient 1, 10% of ingredient 2, and 70% of ingredient 3 resulted in the highest prediction score of five (5); meanwhile, other compositions reached the prediction score of four (4).

3.3 Discussion

In a sensory test, the easiest way to analyze the score is the average score or based on descriptive analysis [21]. In this study, the descriptive method was still successful in finding the best product with the highest average score. Each design point had two replications, each with a different average score. For example, in samples 1A and 1B, the difference between the average scores was 0.53. This different was not significant statistically at α = 5% (t-test, p-value = 0.2163). It means that the taste of the compositions was quite the same. The average score method's weakness is that the effect of each ingredient and its binary blending on the taste can not be investigated. Hence, modeling approaches are used to overcome this disadvantage.

Based on the second-order Scheffé model, Table 5 shows the prediction responses. The prediction responses of the same compositions were the average of two responses. For instance, the average scores of 5A and 5B were 3.820 and 4.600, respectively. Hence, the response prediction of the Scheffé model is 4.210, which is the mean of the two average scores. In this model, the optimum conditions were obtained on two compositions (10%, 20%, 70%) and (30%, 10%, 60%). However, no terms in the model were significant, although R2 was 67%, and the optimum conditions were defined. The optimum condition was (30%, 10%, 60%). The optimum conditions were the same as the average scores.

Table 5. Response prediction of the composition for linear and ordinal models

Run	x1 (%)	x2 (%)	x3 (%)	Average score	Response prediction of the Sheffe model	Response prediction of the ordinal model
5A	0,1	0,1	0,8	3,820	4,210	4
5B	0,1	0,1	0,8	4,600	4,210	4
3A	0,1	0,2	0,7	4,600	4,525	4
3B	0,1	0,2	0,7	4,450	4,525	4
4A	0,1	0,3	0,6	3,730	3,715	4
4B	0,1	0,3	0,6	3,700	3,715	4
6A	0,2	0,1	0,7	3,730	3,910	4
6B	0,2	0,1	0,7	4,090	3,910	4
2B	0,2	0,2	0,6	4,100	4,150	4
2A	0,2	0,2	0,6	4,200	4,150	4
1A	0,3	0,1	0,6	4,800	4,535	5
1B	0,3	0,1	0,6	4,270	4,535	5

The second modeling approach was ordinal logistic regression. As mentioned, the problem in mixture experiments is the multicollinearity between ingredients. Multi-collinearity in regression analysis will affect the parameter estimation. Estimating the model parameters will be a different sign or overestimate or underestimate [22]. [23], [24] addressed the way to handle multicollinearity in logistic regression. However, if the multicollinearity is ignored, the parameter estimation of the third ingredient was zero, and the statistic chi-square reached 10.000. The parameter estimations were reasonable if the model did not involve the third ingredient. Table 3 shows the parameter estimations of the model. The model focused on the binary blending between ingredients one and three because it was statistically significant at $\alpha = 5\%$. Table 5 shows that if ingredient 1 increased, the prediction response also increased if ingredient three decreased. The prediction response's highest value was when ingredient one was maximum, and ingredient three was minimum. This result was related to the hypothesis testing of model coefficients. The two binary blendings were not statistically significant at $\alpha = 5\%$.

The advantage of ordinal logistic regression is that the response's prediction can be defined based on the probability estimation from the model. Based on the coefficient model in Table 3, each composition's probability belongs to a particular score shown in Table 6. The score prediction of a design point or a composition is based on the highest probability among the scores. Almost all design points were predicted to score four, except the composition (30%, 10%, 60%) was predicted to score 5. The result is in line with [20], [25].

Table 6. The probabilities of each design point on each value of ordinal scale

Runs	Prob[1]	Prob[2]	Prob[3]	Prob[4]	Prob[5]	Prob[6]	Most Likely score
1A	0,012	0,009	0,084	0,362	0,456	0,077	5
1B	0,012	0,009	0,084	0,362	0,456	0,077	5
2A	0,027	0,020	0,162	0,455	0,301	0,036	4
2B	0,027	0,020	0,162	0,455	0,301	0,036	4
3A	0,024	0,018	0,150	0,449	0,319	0,039	4
3B	0,024	0,018	0,150	0,449	0,319	0,039	4
4A	0,063	0,045	0,287	0,435	0,155	0,015	4
4B	0,063	0,045	0,287	0,435	0,155	0,015	4
5A	0,019	0,015	0,125	0,427	0,365	0,049	4
5B	0,019	0,015	0,125	0,427	0,365	0,049	4
6A	0,043	0,032	0,229	0,462	0,212	0,022	4
6B	0,043	0,032	0,229	0,462	0,212	0,022	4

4. CONCLUSION

In the sensory test, when the response is a Likert scale, there are three analysis methods. The simple method is the average score. However, the average score method has a weakness: it cannot investigate the effect of each ingredient and its binary blending on the taste. To overcome this, modelling approaches can be chosen. The Likert scale belongs to an interval scale or an ordinal scale. The linear and ordinal logistic regression can be alternatives based on the data response type. Despite the complexity of the modelling, the modelling methods give more insight into the relationship among the ingredients. In this case study, the three methods give the same results for the best ingredients. The ordinal logistic model can identify important factors when the linear model fails to do so. Further research can be expanded to develop methods for overcoming the high multicollinearity in mixture experiments with ordinal responses. In addition, from a mixture experiment point of view, it is also necessary to develop the optimal designs based on ordinal response since they will have different design points

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