Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Chromatography A, 1054 (2004) 39–46
JOURNAL OF CHROMATOGRAPHY A
www.elsevier.com/locate/chroma

Correlating sensory attributes to gas chromatography–mass spectrometry profiles and e-nose responses using partial least squares regression analysis

Tetsuo Aishima*

Chemometrics and Sensometrics Laboratory, 1-197 Sengen-cho, Omiya-ku, Saitama 330-0842, Japan

Available online 11 September 2004

Abstract

Sensory scores for 15 attributes identified in soy sauce aroma by quantitative descriptive analysis were correlated with purge and trap gas chromatography–mass spectrometry (GC–MS) profiles and electronic nose (e-nose) responses using partial least squares (PLS) regression analysis. Highly predictive PLS models were obtained for every attribute based on whole GC–MS profiles. However, the predictability has been greatly improved in the models calculated from 20 selected peaks that showed higher contribution to each attribute in the first PLS analysis. Contrarily, except for *alcoholic* and *fishy* notes, predictability of PLS models calculated from e-nose responses was poor. The correlation between GC–MS profiles and e-nose responses was unsatisfactory due to high similarity in sensor responses.

Keywords: Sensory scores; Electronic nose responses; Partial least squares regression analysis

1. Introduction

In food research and development, quantitative descriptive sensory analysis has widely been used not only in industry but in academia since mid 1970s [1]. The basic principle of this method is very similar to that of chromatographic analysis as schematically shown in Fig. 1 [2]. This similarity gives rational bases for handling obtained sensory data with various statistical techniques that have widely been used in analytical chemistry [3]. In the first step of this sensory method, by using a well trained panel generally composed of 6–15 members, all sensory attributes present in food samples are identified through sniffing, tasting and intensive discussions by panel members [4]. This step may correspond to identification of peak components in gas or liquid chromatographic analysis. In the second step, like quantitative gas chromatographic (GC) or HPLC analysis, each panel member individually quantifies strengths of every attribute identified in samples in the preceding step using a category or line scale. Then, scores given for each attribute by panel members are averaged. Thus, the final form of data is expressed in a two dimensional matrix, m attributes $\times$ n samples.

Although at present no method can accurately illustrate the composition of sample aroma [5]. At the first step of aroma analysis using GC or GC–mass spectrometry (GC–MS), aroma components should be extracted and concentrated from food matrix since generally concentrations of most aroma components contained in food are lower than the detection threshold of detectors. Utilizing volatility and solubility in organic solvent, basic natures commonly shared by aroma components, various extraction and concentration methods have been developed and applied for analysis of food aroma using GC or GC–MS. Among them, simultaneous distillation-extraction (SDE), dynamic headspace analysis or purge and trap method using porous polymer, and solid-phase micro-extraction (SPME) may be the most popularly used methods in aroma analysis [6].

Electric nose (e-nose), a newly coined name indicating an attractive and versatile instrument, was initially developed by combining metal oxide semi-conductor gas sensors in order to mimic the human olfaction system [7,8]. However, the

* Tel.: +81 48 649 6114; fax: +81 48 649 6114.
E-mail address: aishima@chemsensmetrix.com.

0021-9673/$ – see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.chroma.2004.08.056

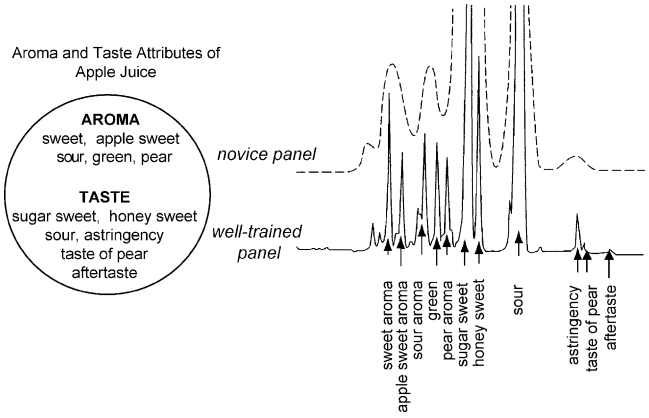

Fig. 1. Schematic presentation for basic principle of descriptive sensory analysis exemplified by apple juice flavor [1].

detection specificity of such gas sensors for gases or aroma compounds was rather poor in nature. Generally, output signals from e-nose have been analyzed by multivariate pattern recognition techniques, such as principal component analysis (PCA) and linear discriminant analysis (LDA). Various successful results to classify the sample "aroma" have been reported since early 1990s [9–12]. However, attempts to correlate e-nose responses to sensory attributes succeeded only partly [13] but should undoubtedly be very important and interesting to develop a new application area of this instrument. Further, if e-nose responses and GC–MS profiles could be statistically correlated each other, analytical results of e-nose might be interpreted on the basis of GC–MS data or chemical information.

Since late 1970s, thanks to an emerging new discipline, chemometrics, in analytical chemistry, sophisticated multivariate data analysis techniques have been applied for sets of matrix data obtained from sensory and/or instrumental analysis of food samples [14,15]. Especially, pattern recognition techniques such as PCA, LDA and SIMCA (soft independent modeling of class analogy) are widely used ones. Further, partial least squares (PLS) regression, currently the most powerful multivariate calibration technique, has been recognized as an indispensable regression technique among analysts working in spectroscopy, chromatography and sensory sciences [16].

The purpose of this research is to compare the predictability of GC–MS profiles and e-nose responses for quantitative descriptive sensory data of soy sauce aroma by applying PLS regression analysis.

2. Materials and methods

2.1. Samples

Fourteen deep-colored type soy sauce samples (A–N) were purchased from a local market in Tokyo. All soy sauce samples were domestic products and produced from soybeans and wheat through the purely fermented process using *Aspergillus* fungi and *Zygosaccharomyces* yeast.

Table 1
Sensory attributes and results of ANOVA

Attribute	Description	*F*	*P*
Sweet	Sweet note of heated sugar	1.87	0.04
Alcoholic	Yeast fermentation note	1.70	0.07
Fruity	Sweet fruity note	1.96	0.03
Sour	Vinegar like note	1.60	0.09
Fermented	Yogurt like note	0.96	0.49
Woody	Pine or cedar wood like odor	2.09	0.02
Roasted	Roasted cereals	1.88	0.04
Boiled bean	Steamed soybean	1.19	0.29
Fishy	Rotten fresh water	1.69	0.07
Gargle	Iodine gargle	1.35	0.19
Medicinal	Medicine like smell	4.22	0.00
Rice bran	Green and a little rancid	1.27	0.24
Dusty	Dusty or earthy	2.06	0.02
Moldy	Odor of molded food	2.37	0.01
Ink	Smell of ink	2.15	0.01

2.2. Sensory evaluation

Quantitative descriptive sensory analysis was applied for evaluating 14 soy sauce samples using a 15 cm line scale by a well-trained panel consisted of 12 members at the age of 30–50, 11 females and one male. They were selected based on their sensitivity for detecting 2-phenylethyl alcohol, skatol, *iso*-valeric acid, γ-undecalactone and cyclotene at their threshold levels (Daiichi-Yakuhin-Sangyo Co., Tokyo Japan) and ability to identify aroma properties of these compounds. Thirty ml of soy sauce was placed in a 180 ml volume of white china cup covered with a plastic petri dish and was served to a panelist at a room temperature, ca. 25 °C. Prior to the quantitative descriptive analysis, 12 panelists had thoroughly discussed aroma properties of samples through three preliminary sessions, each spent 2 h, until all of them had agreed to use them as the attributes. Then, the quantitative descriptive analysis was performed using 15 sensory attributes listed in Table 1 for all 14 samples randomly divided into four sessions, each composed of five, five and four samples. In each session, samples were randomly presented for each panel to avoid causing a so-called order effect. All samples were evaluated once. Every sample was presented to the panel with a three digit random number.

2.3. GC–MS analysis

A 0.5 ml portion of soy sauce sample placed in a 25 ml glass sample purger was heated at 50 °C for 5 min by a sample heater and then purged with He gas at 40 ml/min for 60 min to isolate headspace volatiles, that were adsorbed on a 30 cm × 3 mm i.d. Tenax TA column in a Tekmar LSC2000 (Tekmar Inc., Cincinnati, OH). It was then dry-purged for 30 min with He gas at 40 ml/min to remove water from the Tenax column. The adsorbed compounds were thermally desorbed

at 200 °C for 10 min using He gas at 1 ml/min. Desorbed compounds were cryofocused at the capillary interface maintained at −120 °C with liquid N_2 and then automatically injected on the column by rapidly heating the interface to 220 °C for 2 min.

An HP5971 mass spectrometer connected with an HP5980 gas chromatography (Agilent Technologies, Palo Alto, CA) was used with a DB–WAX (60 m × 0.25 mm, film thickness: 0.25 μm, J&W Scientific Inc., Folsom, CA) fused silica capillary column. The oven temperature was elevated from 50 to 200 °C at 3 °C/min. The flow rate of He used for carrier gas was 1.0 ml/min. GC–MS was operated with an ionization voltage at 70 eV and ion source temperature at 180 °C. All samples were analyzed once. Peak components were identified by matching their mass spectra with those in the Wiley Library of MS spectra (Agilent Technologies) and based on their retention indices. Areas of each peak integrated by an attached computer were used as variables for statistical analysis.

2.4. E-nose analysis

A FOX 4000 e-nose from Alpha-MOS (Toulouse, France), with 18 metal oxide semiconductor gas sensors, was used. The metal oxide sensors may be either n- or p-type, the former respond to oxidizing compounds and the latter to reducing compounds. One ml of soy sauce sample was placed in a 10 ml volume of vial and heated at 50 °C. One ml of headspace air was automatically injected into the e-nose by a syringe and sensor responses were recorded for 120 s. The maximum response points automatically recorded for each of 18 sensors were used as the e-nose response.

2.5. Statistical analysis

Analysis of variance (ANOVA) and PCA were carried out by Senstools 3.1 (OP&P, Utrecht, The Netherlands). PLS analysis was performed by Unscrambler ver.7.01 (CAMO ASA, Trondheim, Norway). The correlations between scores of individual attributes and GC–MS profiles or e-nose responses were analyzed by PLS1 but PLS2 was applied to illustrating correlations between whole sensory, GC–MS and e-nose data sets. All variables, such as GC–MS peak areas, sensor responses and scores of sensory attributes, were *z*-transformed so as to make each variable has a unit variance and zero mean before applying PLS analyses in order to obtain unbiased contribution of each variable to the criterion, *Y*. By applying PLS analysis to *z*-transformed data, importance of peaks for each attribute could be compared quantitatively based on regression coefficients and loading weights for each predictor or *X* variable used in PLS models [17]. After PLS analysis performed with the whole GC–MS data, 20 GC–MS peaks that showed larger absolute magnitude of importance, regardless of signs, were selected as influential ones and the second PLS analysis was performed. In order to examine the robustness of calculated PLS models, estimated

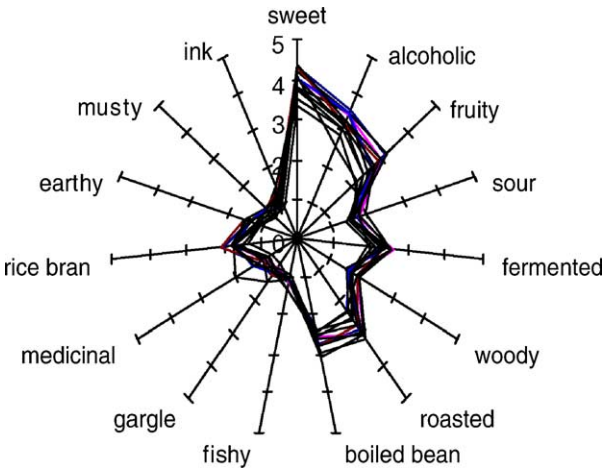

Fig. 2. Comparison of sensory profiles composed of average scores of 15 attributes identified in soy sauce aroma.

scores obtained from cross-validation were compared with scores ordinarily estimated from PLS models. In the cross-validation, a PLS model is calculated after a group of samples has been removed and sensory scores are estimated using the PLS model obtained from the residual samples. Next, a new group of samples has been removed and a PLS model is calculated using the residual samples. This step is continued until all samples removed once [18].

3. Results and discussion

3.1. Sensory analysis

Table 1 shows 15 attributes identified by the panel for describing soy sauce aroma and the resulting sensory scores in eight attributes, such as sweet, fruity, woody, roasted, medicinal, dusty, moldy and ink, were significantly different ($p < 0.05$) among samples. The sensory profiles of 14 samples

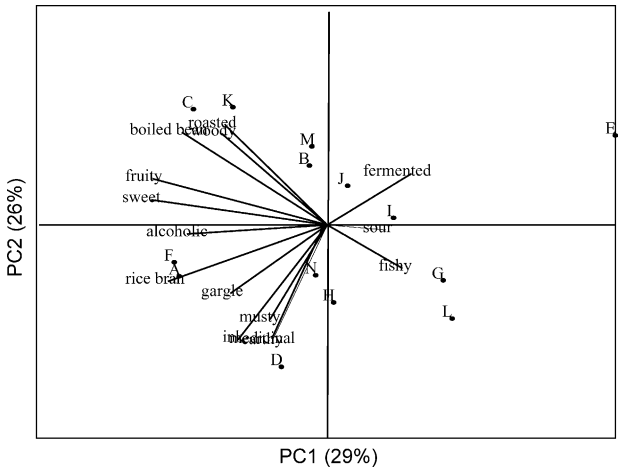

Fig. 3. Factor loadings and principal component scores extracted from descriptive sensory data.

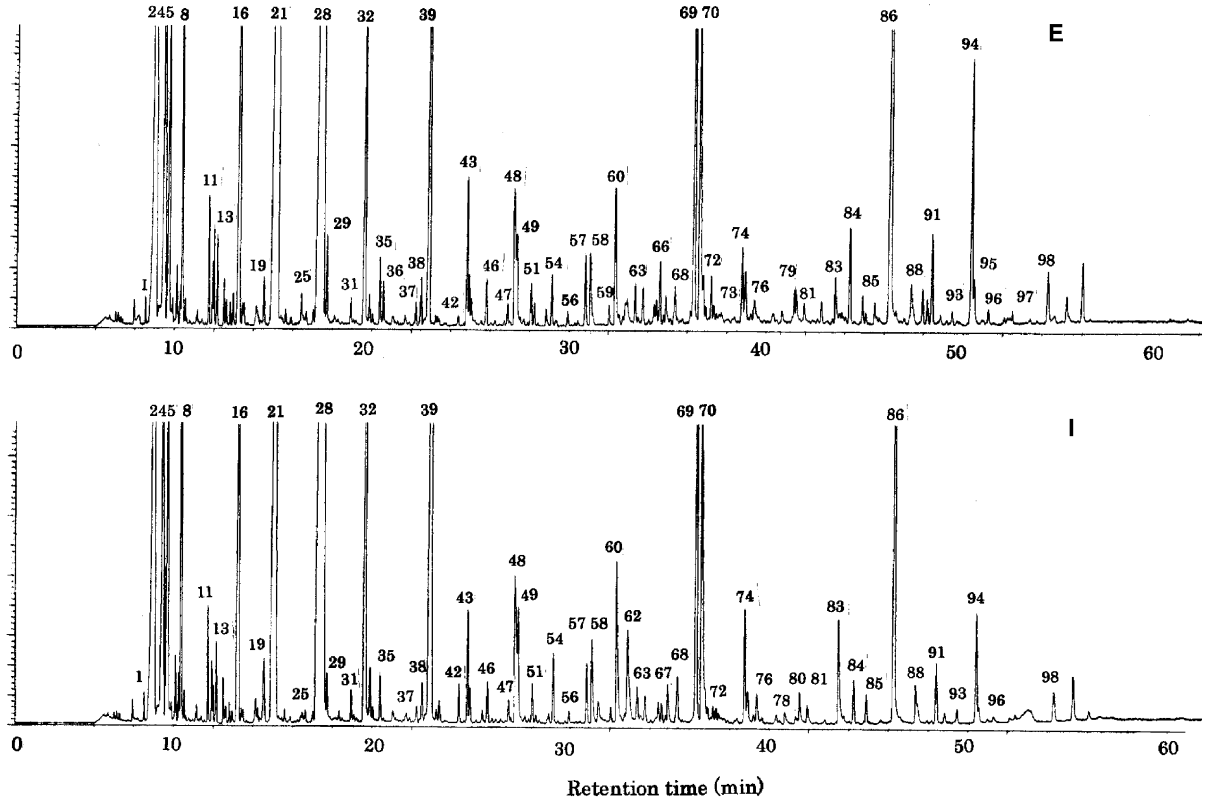

Fig. 4. Purge and trap GC–MS profiles of soy sauce aroma. Numbered 98 peaks were used as predictor variables for PLS regression analysis.

were compared in Fig. 2. A biplot, a scatter plot for scores and factor loadings obtained from PCA, illustrates mutual relationships between samples and attributes (Fig. 3). This biplot suggests that samples may be classified into four or five groups on the basis of aroma characteristics. As easily assumed from only three attributes, *sour*, *fermented* and *fishy* locating in the right side, the uniqueness of *E* is derived from weakness in most attributes.

3.2. Sensory data vs. GC–MS data

More than 120 peaks were observed in purge and trap GC–MS profiles but 98 peaks commonly found in all 14 samples were used as predictor variables, *X*, in the subsequent PLS analysis (Fig. 4). As presented in Table 2 , all contributing proportions, $R^2 \times 100$, calculated for every attribute based on PLS models surpassed 76%. These higher values clearly indicate that all attributes identified in soy sauce aroma have strong correlations with headspace GC–MS profiles as already found in soy sauce aroma using linear multiple regression analysis [19,20]. It has already been shown in our previous works on aromas of seafood and fish that the predictability could be improved by calculating a new PLS model using a set of selected peaks that had shown higher contributions for estimating *Y* [21,22]. Further, it could be much easier to examine the relationships between each attribute and chemical components, if the PLS model would be calculated from a smaller number of peaks. Therefore, 20 highly contributing peaks were chosen from 98 peaks by comparing importance in a PLS model in order to obtain a more comprehensive and higher predictive PLS model. As Table 2 clearly indicates, the predictability for each attribute has been greatly improved in the PLS model composed of 20 peaks selected through the aforementioned step. As shown in Fig. 5, close relationships between *alcoholic* scores from sensory evaluation and those estimated by the 20-peak PLS model were

Table 2
Contributing proportions ($R^2 \times 100$) in PLS models calculated from whole GC–MS peaks, selected 20 peaks, and 18 gas sensors in electronic nose

Attribute	$R^2 \times 100$		
	GC–MS		Electronic nose 18 gas sensors
	98 peaks	20 peaks	
Sweet	87	97	9
Alcoholic	89	98	51
Fruity	90	97	17
Sour	82	96	12
Fermented	81	90	13
Woody	86	93	16
Roasted	90	96	2
Boiled bean	86	98	9
Fishy	90	91	52
Gargle	77	90	9
Medicinal	76	91	20
Rice bran	81	96	17
Earthy	96	95	38
Musty	78	94	22
Ink	76	94	7

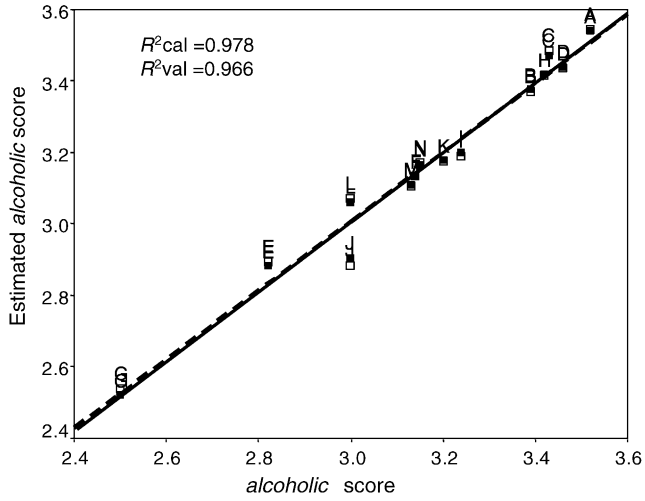

Fig. 5. Relationships between sensory scores for *alcoholic* and scores estimated based on the PLS model calculated from GC–MS profiles. Solid line: observed scores vs. scores estimated by calibration model (■), dotted line: observed scores vs. cross-validated scores (□). R^2cal: contributing proportion in calibration *model*, R^2val: contributing proportion in cross-validation.

indicated in both ordinary and cross-validated estimations. Thus, the PLS model calculated for *alcoholic* using highly contributing 20 peaks was a robust one.

Fig. 6 shows a scatter plot of factor loadings on 20 peaks and *alcoholic* in the first and second PLS components. The importance of each peak for *alcoholic* can be quantitatively compared on this plot as described below [23]. At first, draw a line from the point of *alcoholic* through the origin (0, 0) and through to the other side from the origin. A perpendicular line drawn from the *i*th GC–MS peak on this line projects the *i*th peak point onto the line. The length of the projection or *i*th peak point to the origin (0, 0) is proportional to importance of *i*th peak for *alcoholic*. For example the peak 16: *iso*butyl alcohol should be more important than peak 19: 2-pentanol

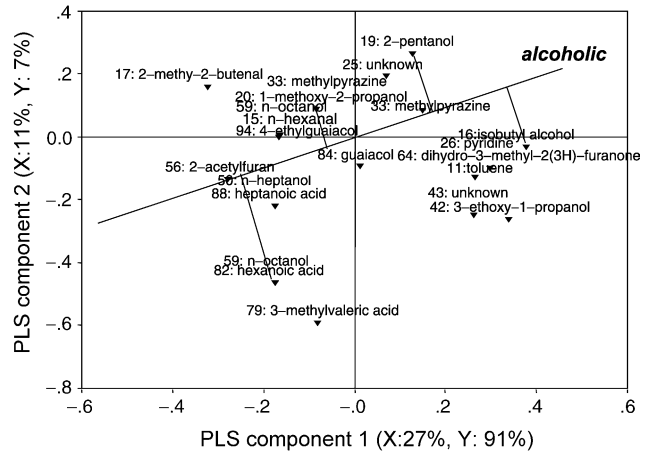

Fig. 6. Factor loadings of PLS components 1 and 2 on selected 20 GC–MS peaks and *alcoholic* for calibrating *alcoholic* scores. See the text for interpretation of this figure.

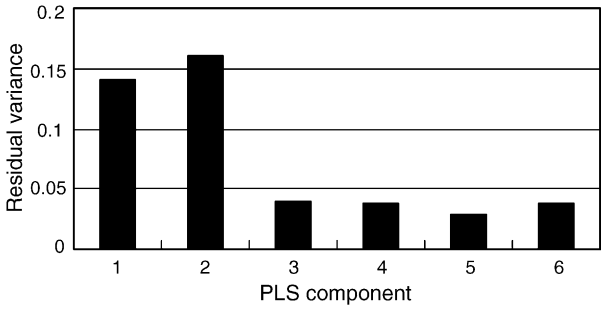

Fig. 7. Changes in residual variance in relation to the number of components constructing PLS models. The five-component PLS model is the best since the residual variance attains smallest there.

because the length from origin to the peak16 point is much longer than that from origin to the peak 19 point. That is, in Fig. 6, peaks closely locating to *alcoholic*, such as 16: *iso*butyl alcohol, 64: dihydro-3-methyl-2(3*H*)-furanone and 19: 2-pentanol are highly contributed to *alcoholic* but peaks in the opposite side, such as 56: 2-acetylfuran, 82: hexanoic acid and 79: 3-methylvaleric acid, are contrarily contributing or weakening the *alcoholic* note. However, examining relationships between each attribute and chemical components, their importance suggested by PLS analysis, is another research subject and so detailed comments are refrained here.

The optimum number of PLS components to obtain the most accurate prediction could be decided by comparing residual variances obtained from cross-validation. As Fig. 7 shows, the lowest residual variance was attained at the five-component PLS model but R^2 (0.978) obtained from the two-component PLS model was high enough as already shown in Fig. 5. Further, if we consider the predictability and easiness in the interpretation of PLS model, the two-component PLS model may have some advantage over the five-component PLS model because of its simple structure.

3.3. Sensory data vs. e-nose data

According to Table 2, contributing proportions calculated from PLS models using e-nose responses as predictors surpassed 50% only for *alcoholic* and *fishy* notes but those for all other 13 attributes were much smaller. Comparing residual variances calculated from cross-validation, the six-component PLS model with R^2 = 0.877 was the best for predicting *alcoholic*, however, R^2 from the cross-validation was only 0.508 (Fig. 8). It means that only a half of variation contained in *alcoholic* scores could be explained even by this best PLS model. However, 100% variance in sensor responses had already been extracted in the first two PLS components (Fig. 9). We may naturally wonder what kind of information could be contained in the additional four PLS components since the most of principal information has already been extracted into the first two PLS components. The factor loading plot shown in Fig. 9 indicates that 18 gas sensors are classified into contrasting two groups, 5 sensors (SY/AA, SY/G, SY/gCTI, SY/Gh and SY/gCT) characterized with negative

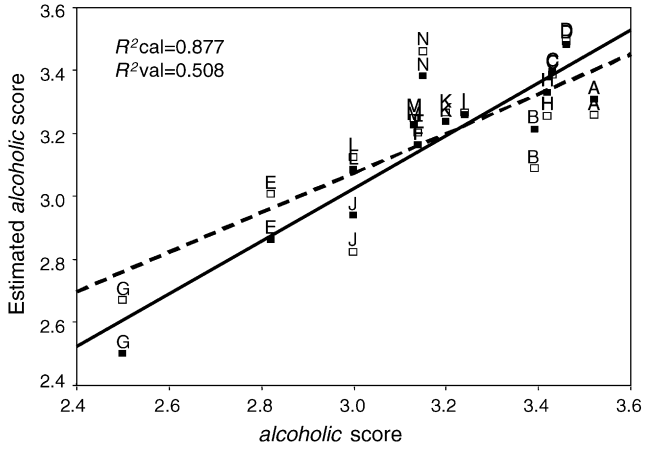

Fig. 8. Relationships between observed sensory scores for *alcoholic* and scores estimated based on the six-component PLS model calculated from e-nose responses. Solid line: observed vs. scores estimated from calibration model composed of six PLS components (■), dotted line: observed vs. cross-validated scores (□). R^2cal: contributing proportion in calibration *model*, R^2val: contributing proportion in cross-validation.

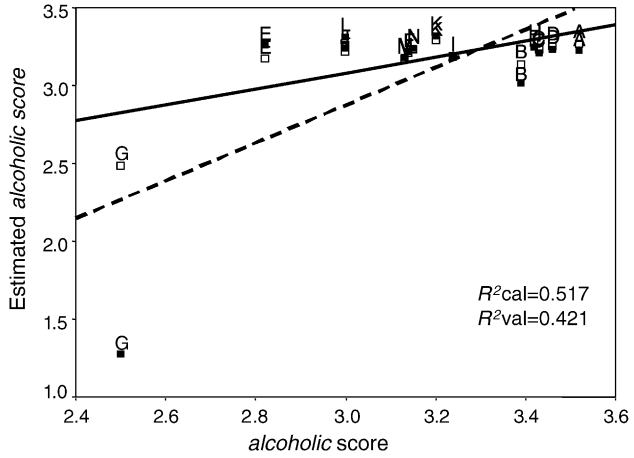

Fig. 10. Relationships between observed sensory scores for *alcoholic* and scores estimated based on the two-component PLS model calculated from e-nose responses. Solid line: observed vs. scores estimated from the calibration model composed of two PLS components (■), dotted line: observed vs. cross-validated scores (□). R^2cal: contributing proportion in calibration *model*, R^2val: contributing proportion in cross-validation.

factor 1 loadings and other 13 sensors with positive factor 1 loadings. This clear classification may simply reflect two types, n and p, of gas sensors installed in the e-nose but further comments cannot be made because detailed information on features in these sensors has not been supplied from the manufacturer. Although nearly 100% variance has already been extracted into the first two PLS components, predictability of the model was unsatisfactory and not robust as the great differences between calibrated and cross-validated scores indicate (Fig. 10). Thus, at present, e-noses, regardless of using any sensors currently available, may not be able to supply information relevant to sensory attributes in food aroma as Morvan et al. [13] have already reported using a MOS-MOSFET gas sensor array.

Next, exactly opposite arrangement of sensors shown in Fig. 9 was obtained from PLS analysis for *fishy* and sensor responses. As Fig. 11 shows, five sensors (SY/gCT, SY/gCTI, SY/Gh, SY/G and SY/AA) locate in the positive side but other 13 sensors are placed in the negative side in the factor loading plot. Two contrasting classification shown in Figs. 9 and 11 may correspond to widely known fact that different groups of aroma compounds are responsible for *alcoholic* and *fishy* notes. Generally, alkyl amines cause the *fishy* note but the *alcoholic* note is usually derived from alcohols and aldehydes.

3.4. Whole sensory data vs. whole e-nose data

To examine overall relationships between whole attributes and whole sensor responses, two data sets were analyzed by PLS2. Fig. 12 shows a first and second factor loading plot for attributes and sensors with sample scores superimposed. As this plot indicates, as already found in Figs. 9 and 11, 18 sensors were classified into two groups each composed of 5

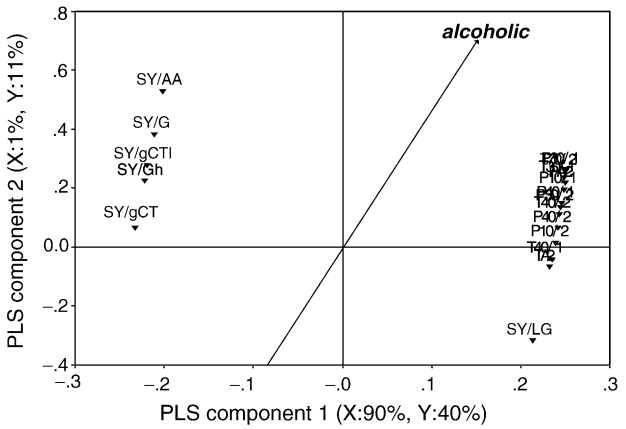

Fig. 9. Factor loadings of PLS components 1 and 2 on 18 gas sensors and *alcoholic*.

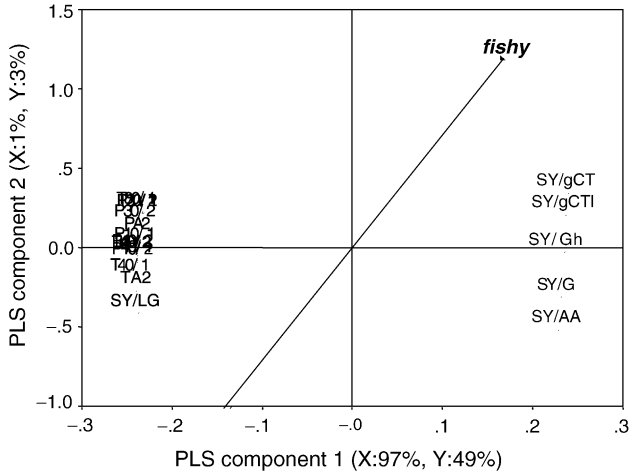

Fig. 11. Factor loadings of PLS components 1 and 2 on 18 gas sensors and *fishy*.

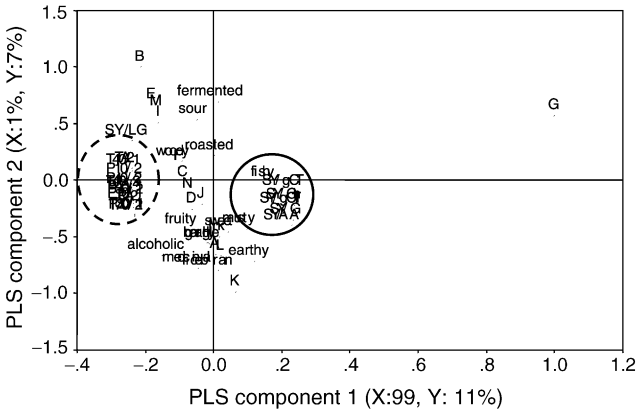

Fig. 12. Factor loadings of PLS components 1 and 2 on 15 sensory attributes and 18 gas sensors.

SY sensors and other 13 sensors. Examining sample distribution, G seems somewhat different from other soy sauce but uniqueness of this sample has not been indicated in the PCA plot obtained from sensory scores (Fig. 3). Although the first PLS component account for 99% of variance contained in sensor responses, the sensory related variance extracted was only 11% due to the complicated mature of food aroma and too simple specificity in sensor responses. Until now the total number of aroma compounds identified in food has surpassed 7000 [24] and most food aromas except for certain fresh vegetables and fruits are derived from complicated mixtures of various aroma compounds [25].

3.5. GC–MS data vs. e-nose data

Relationships between whole e-nose responses and whole GC–MS profiles were analyzed by PLS2. Fig. 13 shows a first and second factor loading plot for 98 GC–MS peaks and 18 sensors with sample scores superimposed, where two sensor clusters, one composed of 5 SY sensors and another of other 13 sensors, locate in the opposite sides and 98 GC–MS peaks are placed in between. The contributing proportion attained to 93% (=89 + 4) by the first two PLS components but this large proportion seems to be simply derived by two sensor groups placed in the opposite sides. Further, only a few GC–MS peaks seem to have significant correlation with sensors. Although a large variation, 89%, was extracted in the first PLS component, most variation seemed irrelevant to sensory characteristics since 13 samples except for G were simply arranged vertically. Thus, this 89% may simply reflect variation contained in volatiles of soy sauce samples but not closely related to sensory properties.

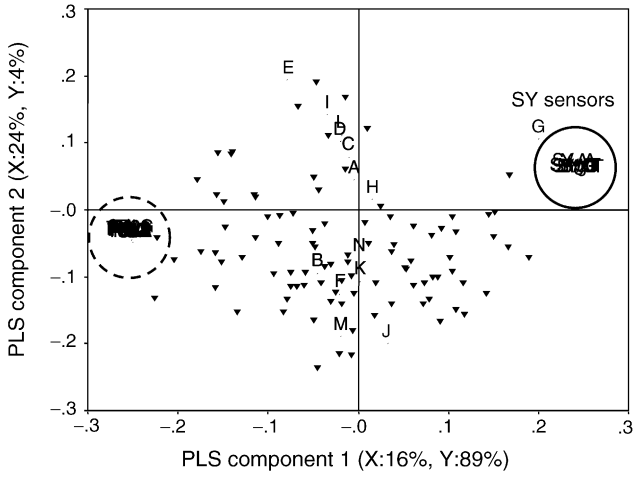

Fig. 13. Factor loadings of PLS components 1 and 2 on 98 GC–MS peaks (▼) and 18 gas sensors.

4. Conclusions

Fifteen attributes developed for describing soy sauce aroma were useful to differentiate 14 brands of soy sauce distributed in Japan. Each of 15 descriptive sensory attributes could be well correlated to GC–MS profiles by PLS regression analysis. Calculating PLS models with 20 peaks highly contributed for predicting each attribute has greatly improved the predictability of models and interpretation of the meanings implied in them. On the other hand, predictability of e-nose responses for sensory attributes was unsatisfactory except for *alcoholic* and *fishy*, due to poor response specificity and diversity in gas sensors installed in the e-nose. According to the PLS loading plot, it was assumed that two groups of sensors having highly similar response properties are installed in the e-nose because 18 gas sensors were classified into two groups both tightly clustered 5 and 13 sensors. These results indicated that novel gas sensors carrying higher specificity and wider diversity should be created to construct a capable and reliable future e-nose to correlate its responses to sensory data.

References

[1] H. Stone, J. Sidel, S. Oliver, A. Woolsey, R.C. Singleton, Food Technol. 28 (11) (1974) 24.
[2] T. Aishima, Food Chem. Monthly 15 (1) (2002) 26 (in Japanese).
[3] B.G.M. Vandeginste, D.L. Massart, L.M.C. Buydens, S. DeJong, P.J. Lewi, J. Smeyers-Verbekem, Handbook of Chemometrics and Qualimetrics: Part B, Elsevier, Amsterdam, 1998, p. 421.
[4] M.C. Meilgaard, G.V. Civille, B.T. Carr, Sensory Evaluation Techniques, third ed., CRC Press, Boca Raton, FL, 1999, p. 161.
[5] M.M. Leahy, G. Reineccius, in: P. Schreier (Ed.), Analysis of Volatiles, DeGruiter, Berlin, 1984, p. 19.
[6] G. Reineccius, in: A.J. Taylor (Ed.), Flavour Technology, Shefield Academic Press, Shefield, 2002, p. 210.
[7] T. Aishima, Anal. Chim. Acta 243 (1991) 293.
[8] J.W. Gardner, H.V. Shurmer, T.T. Tan, Sens. Actuators B 6 (1992) 71.
[9] T. Aishima, J. Agric. Food Chem. 39 (1991) 752.
[10] H. Ulmer, J. Mitrovics, G. Noetzel, U. Weimer, W. Göpel, Sens. Actuators B 43 (1997) 24.
[11] C.D. Natale, A. Macagnano, E. Martinelli, E. Proietti, R. Paolesse, L. Castellari, S. Campani, A. D'Amico, Sens. Actuators B-Chem. 77 (2001) 61.

[12] A.M. Taurino, D.D. Monaco, S.C.M. Epifani, R.R.P. Siciliano, L. Ferrara, G. Maglione, A. Basso, D. Balzarano, Sens. Actuators B-Chem. 95 (2003) 123.
[13] M. Morvan, T. Talou, J.-F. Cois Beziauc, Sens. Actuators B-Chem. 95 (2003) 212.
[14] M. Forina, S. Lanteri, C. Armanino, Curr. Chem. 141 (1987) 93.
[15] T. Aishima, S. Nakai, Food Rev. Int. 7 (1991) 33.
[16] H. Martens, T. Naes, Multivariate Calibration, Wiley, Chichester, 1989.
[17] The Unscrambler User Manual, CAMO ASA, Trondheim, 1998, p. 273.
[18] M.A. Sharaf, D.L. Illman, B.R. Kowalski, Chemometrics, Wiley, Chichester, 1986, p. 254.
[19] T. Aishima, A. Nobuhara, Food Chem. 2 (1977) 81.
[20] T. Aishima, in: G. Charalambous, G. Inglett (Eds.), Instrumental Analysis of Foods, Academic Press, New York, 1983, p. 37.
[21] K. Morita, K. Kubota, T. Aishima, Food Chem. 78 (2002) 38.
[22] K. Morita, K. Kubota, T. Aishima, J. Sci. Food Agric. 83 (2003) 289.
[23] S. Wold, in: H. van de Waterbeemd (Ed.), Chemometric Methods in Molecular Design, VCH, Weinheim, 1995, p. 195.
[24] L.M. Nijssen, C.A. Visscher, H. Maarse, L.C. Willemsens, M.H. Boelens, Volatile Compounds Found in Food, seventh ed., TNO Nutrition and Food Research Institute, Zeist, 1996.
[25] H.E. Nursten, D.G. Land, H.E. Nursten (Eds.), Progress in Flavour Research, Applied Science, London, 1979, p. 337.