Prediction of Cooked Rice Texture Using an Extrusion Test in Combination with Partial Least Squares Regression and Artificial Neural Networks

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ABSTRACT

Spectral stress strain analysis was used in combination with partial least squares (PLS) regression and artificial neural networks (ANN) to predict nine sensory texture attributes of cooked rice. The models calculated with ANN were significantly more accurate in predicting most of the sensory texture characteristics evaluated than the PLS models. Furthermore, ANN models were more robust and discriminative than PLS models.

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Correlations between instrumental mechanical tests and sensory evaluation techniques of cooked rice texture have been evaluated using multivariate regression (Meullenet et al 1998, 1999). Previous study by Meullenet et al (1999) showed that sensory texture characteristics of cooked rice were successfully predicted using spectral stress strain analysis (SSSA), a spectral analysis of the force deformation curve, and partial least squares (PLS) regression along with an extrusion test. However, the use of multivariate regression is limited by the necessity of the human's understanding in describing rules to a computer or a software (Bomio 1998). Artificial neural networks (ANN) were developed almost four decades ago as a tool that has the ability to handle information-processing problems (Ni and Gunasekaran 1998). ANN have recently gained more attention because of advanced technology in computer hardware and software (Bomio 1998). ANN consist of instant patterns of recognition with hidden rules. A network normally consists of a succession of layers with connections between layers (Ni and Gunasekaran 1998). Data are introduced to the network as the input layer and the response of the given input transfers to an output layer. Hidden layers between input and output, connected with adjustable weights, transfer the internal information of input to a latent output (Ni and Gunasekaran 1998).

ANN are capable of handling data with nonlinear relationships even though the precise manner of those relationships is not known. ANN are also suitable for food quality prediction, which, in many instances, is complicated due to interrelationships among quality parameters, composition, and processing conditions (Ni and Gunasekaran 1998). Multiple linear regression is widely used for correlating instrumental measurements to texture perception of foods; however, the relationships between dependent variables and independent variables must be either linear or simple. Hence, ANN could be useful in elucidating the complex relationship between the sensory perception of cooked rice texture and instrumental measurements. The aims of this study were 1) to further investigate the use of SSSA as a means of predicting sensory texture characteristics of cooked rice and 2) to compare PLS regression and ANN as two modeling techniques.

MATERIALS AND METHODS

Samples

Three rice cultivars, two long-grain (Cypress and Kaybonnet) and one medium-grain (Bengal) harvested from Stuttgart and Dewitt, AR, in 1996 and 1997 were used in this study. Rice samples were collected from the University of Arkansas Rice Research and Extension Center in Stuttgart (1996) and a farm in Dewitt (1997). Rice samples were immediately brought to the University of Arkansas Rice Processing Laboratories and cleaned using a Carter-Day Dockage Tester (Carter-Day Co., Minneapolis, MN). Samples were stored in airtight plastic buckets at –10°C for approximately one month. Samples then were dried and stored under various storage moisture contents (10–12%) at various temperatures (4–38°C). Samples were pulled for evaluation after various storage durations (0–52 weeks). A partial factorial design was used for both harvest years with a total number of observations of 74 in 1996 and 56 in 1997. More details about the processing treatments can be found in Sitakalin and Meullenet (2000).

Stored samples were allowed to equilibrate to room temperature before hull and bran were removed. A McGill sample sheller (husker) and a McGill No. 2 mill were used to remove the hull and bran, respectively. Samples were milled to a constant degree of milling (DOM = 90). A Satake Milling Meter MM-1B was used for measuring the DOM.

Sensory Evaluation

Rice samples were cooked in a household rice cooker with a rice-to-water ratio of 1:2 (v/v) and served to panelists in preheated glass bowls at 75 ± 2°C. Panelists were instructed to monitor temperature closely during the tests and taste rice samples before the temperature of samples reached 60°C. Complete sample preparation and sensory evaluation procedures are given in Meullenet et al (1998, 1999).

Nine panelists with three years of experience and trained in descriptive analysis techniques according to the Spectrum methodology (Sensory Spectrum, Chatham, NJ) evaluated and scored eight texture attributes of cooked rice. Four 3-hr orientation sessions were held for the panelists to develop the rice lexicon and test technique for each attribute evaluated. The nine texture attributes were evaluated during four evaluation stages: surface characteristic, first bite, chew down, and residual stage. Attributes were evaluated at each stage; definitions are given in Table I. Panelists used paper ballots and values 0–15 (Meilgaard et al 1991) to record sensory scores. References were provided to panelists to use as anchors for specific attributes. A list of references used is provided in Sitakalin and Meullenet (2000).

Extrusion Cell Test

Samples were prepared according to the procedures described by Meullenet et al (1998, 1999). An extrusion test, using 35 g of cooked rice at room temperature, was performed using a cylindrical extrusion cell (40 mm in diameter and 70 mm deep) in conjunction with a texture analyzer (model TA-XT2, Texture Technologies Corp., Scarsdale, NY) and procedures described by Meullenet et al (1999). A 25-kg maximum-load load cell was used and the crosshead speed was set to 5.0 mm/sec for a total travel of 55 mm, as previously reported by Meullenet et al (1999). Data were collec-

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ted using the X-TRAD software (v. 3.70). The force in Newtons (N) required to extrude the sample was recorded as a function of time, and six repeated measures were performed on each sample.

Data Analysis

Means for each sensory texture attribute for each sample were calculated. The average force-deformation curve for each sample was exported to a spreadsheet software (Microsoft Excel 97). A multivariate analysis software, Unscrambler (v. 6.11a; CAMO, Trondheim, Norway) was used to determine predictive models of texture attributes. Means for sensory data and force-deformation curves were exported to Unscrambler. Points extracted from the force-deformation curve (i.e., 217 points) were used as variables in regression model to predict each sensory attribute, a procedure known as SSSA (Meullenet et al 1999).

Two sets of data (training and test sets) were required to perform ANN. The training set was used for the network learning process, whereas the test set was used to validate the results. Test sets for each sensory attribute were created using rice samples from an extrusion test performed on samples from both harvest years. Each test set consisted of 30 manually selected samples based on results from preliminary studies using the PLS regression with full cross-validation method (data not shown). Samples in the test set were selected for each sensory attribute from the plots between predicted and measured sensory scores (PLS). The plots were divided into three regions (low, medium, and high), and 10 samples from each region were selected. The remaining 100 samples were used as the training set. Test and training data sets were first fitted by PLS regression using the test set validation method and the PLS1 option of the Unscrambler (CAMO). Instrumental data were weighted by standard deviation so that each instrumental variable was given the same chance to influence the predictive models. The regression models were then exported to a file format compatible with the ANN software. Neural Unscrambler (v. 1.02; CAMO ASA, Trondheim, Norway), software for multivariate calibration applying ANN, was used in the next step to determine predictive models for texture attributes and to compare ability in predicting sensory texture attribute of cooked rice with PLS regression.

The two steps involved in ANN modeling were calibration (training) and prediction. In the calibration (training) step, weights for every neuron in the network were determined. The weights were adjusted from the prediction error using the back-propagation rule. A set of data from the training set was randomly introduced to the network one by one. The weights (regression coefficients) were updated every time to make the prediction error as small as possible. After completion of the network training, the test sample set was presented to the model for prediction.

Networks evaluated in this study consisted of an input layer (with several input nodes), two hidden layers, and one output layer (sensory attribute). Theoretically, the optimal number of principal components (PC) suggested by the PLS regression is used as the number of nodes in the input layer. Hence, there is one input node for each significant principal component. ANN, to be successful in predicting the output variable, must include as many necessary input nodes as possible. However, at the same time, the model has to contain as few unnecessary input elements as possible to reduce noise and overfitting. In this study, three architectures were designed and used for each sensory attribute evaluated. The first architecture was designed with the number of nodes in the input layer equal to the number of principle components suggested for the PLS regression models using the test set method. The number of nodes in the input layer for the second architecture was selected to be equal to the number of principle components suggested by PLS regression for the full cross-validation method. Two hidden layers for these two architectures consisted of one with four hidden neurons and one with two hidden neurons. The third architecture was designed to have four input nodes with two hidden layers (one with three neurons and one with two neurons) and one output layer. This last architecture was tested to represent a simple network with a small number of input nodes. The number of iterations, which is the number of times the weights were updated, was set at 20,000. The learning rate, the size of the weight changes during training, was equal to 1.0. Number of runs or number of calibrations and number of objects shown to the network before the weights were updated were set at 10.

Root mean square error of prediction (RMSEP), the average difference between predicted and measured response values, was used to express the predictive ability of each model in the same unit as the original response variable (sensory score). RMSEP values for the test set method from PLS regression models were compared with the values from ANN and reported in terms of percent improvement. The ratio of RMSEP and RMSE of calibration (RMSEP/RMSEC) was calculated and used as an indication of model robustness. A ratio close to 1 indicates a robust model. Furthermore, a ratio of the standard deviation of a sensory attribute (S_{tot}) and RMSEP was calculated to indicate model discrimination ability. Models with a large ratio (≥2) were considered to be discriminative.

RESULTS AND DISCUSSION

All sensory attributes evaluated except for cohesiveness of mass evaluated after three chews (R_c = 0.43, Table II) were successfully predicted using PLS regression (test set validation method). In all cases, the ANN models (Table III) were improved over the models obtained from PLS regression.

Predictive models for adhesiveness to lips from ANN with a (8, 4, 2, 1), a (7, 4, 2, 1), and a (4, 3, 2, 1) architecture (RMSEP = 0.463, 0.445 and 0.456, respectively, Table III) were better than the model obtained by PLS regression (RMSEP = 0.588, Table II). The RMSEP from ANN was improved by at least 21.3% (Table III). The most robust model from ANN consisted of seven input parameters (ANN [7, 4, 2, 1]) (RMSEP/RMSEC = 1.00, RMSEP = 0.445, S_{tot}/RMSEP = 3.99). The models with a higher number of input nodes (ANN [8, 4, 2, 1]) were less robust (RMSEP/RMSEC = 1.37). The best model (ANN [7, 4, 2, 1]) was also slightly better in predicting adhesiveness to lips in comparison to PLS regression model (RMSEP = 0.46) reported by Meullenet et al (1999).

The prediction of hardness was also improved by 7.8 to 12.3% using ANN with three different architectures. The most robust model was acquired when using a (4, 3, 2, 1) architecture (RMSEP/RMSEC = 1.09, Table III). Furthermore, RMSEP for this model (RMSEP = 0.326) was lower than the value acquired from PLS regression (RMSEP = 0.359, Table II). However, the RMSEP for the best model (ANN [4, 3, 2, 1]) (RMSEP = 0.326) was higher than that reported by Meullenet et al (1999) using PLS regression (RMSEP = 0.19). The larger number of samples used in the present study (n = 130) might result in a higher RMSEP value than that reported by Meullenet et al (1999; n = 74). This hypothesis is confirmed by the fact that the R_c value reported here (R_c = 0.96, Table III) is greater than that reported by Meullenet et al (R_c = 0.81) Although the RMSEP value was lowest and the model most discriminative when using a (6, 4, 2, 1) architecture (RMSEP = 0.315, S_{tot}/RMSEP = 2.47), overfitting was likely (RMSEP/RMSEC = 2.03, Table III). In other words, the model was overly complex for the response in this data set. Thus, the model with four input nodes was chosen as the model best suited for future predictions.

Prediction of cohesiveness of mass evaluated after three chews dramatically improved by 28.5 to 41.6% (Table III) when using an ANN. The number of principle components suggested by PLS regression (test set validation method) was one. Hence, ANN with input nodes equal to number of PC suggested by PLS regression (ANN [1, 4, 2, 1]) was not performed. The RMSEP value of the test set using PLS regression was 1.25 (Table II), whereas it was reduced to 0.73 with a (4, 3, 2, 1) architecture and 0.893 with a (2, 4, 2, 1) architecture. Models from both ANN architectures were very robust (RMSEP/RMSEC = 1.01 and 1.09, Table III). How-

TABLE I
Vocabulary for Sensory Textural Attributes of Cooked Rice

Term	Definition	Technique
Surface		
Adhesiveness to lips	Degree to which sample adheres to lips.	Compress sample between lips, release, and evaluate.
Particle size	Amount of space the particle fills in themouth.	Place sample in center of mouth and evaluate.
First chew		
Hardness	Force required to compress the sample.	Compress or bite through sample with molars or incisors.
Chewdown		
Cohesiveness of mass (3 chews)	Degree to which chewed sample holds together.	Chew sample with molar teeth up to 3 times and evaluate.
Cohesiveness of mass (8 chews)	Degree to which chewed sample holds together.	Chew sample with molar teeth 8 times and evaluate.
Roughness of mass	Amount of roughness perceived in chewed sample.	Chew sample with molar teeth 8 times and evaluate.
Toothpull	Force required to separate jaws during mastication.	Chew sample up to 3 times and evaluate.
Residual		
Toothpack	Amount of product packed into crowns of the teeth after mastication.	Chew samples up to 8 times, expectorate, and feel the surface of the crowns of the teeth with tongue.
Loose particles	Amount of particles remaining in and on the surface of the mouth after swallowing.	Chew sample up to 8 times with molars, swallow and evaluate.

TABLE II
Models Statistic for Partial Least Squares Regression Using the Test Set Validation Method

Sensory Attributes	PC[a]	R_p[b]	RMSEP[c]	R_c[d]	RMSEC[e]	RMSEP/RMSEC
Adhesiveness to lips	8	0.83	0.588	0.87	0.477	1.23
Hardness	8	0.84	0.359	0.91	0.219	1.64
Cohesiveness of mass (after 3 chews)	1	0.38	1.250	0.44	1.057	1.18
Cohesiveness of mass (after 8 chews)	5	0.64	0.614	0.78	0.364	1.69
Roughness of mass	7	0.80	0.227	0.84	0.168	1.35
Toothpull	7	0.88	0.356	0.86	0.305	1.17
Particle size	2	0.56	0.091	0.59	0.076	1.20
Toothpack	5	0.70	0.438	0.88	0.231	1.90
Loose particles	8	0.86	0.437	0.88	0.401	1.09

[a] Number of principle components chosen in regression model explains most of the variation in sensory attributes.
[b] Correlation for the prediction (test set) model (n = 30).
[c] Root mean square error of prediction.
[d] Correlation for the calibration model (n = 100).
[e] Root mean square error of calibration.

ever, the ANN models were not extremely discriminative (S_{tot}/RMSEP = 1.84 and 2.26). Cohesiveness of mass evaluated after eight chews was fairly successfully predicted using ANN (RMSEP = 0.538, 0.513, and 0.573, Table III). The RMSEP values were lower than the values obtained using PLS regression (RMSEP = 0.614, Table II), with improvements between 6.7 and 16.5%. However, the RMSEP values were higher than that reported by Meullenet et al (1999) using PLS regression with random cross-validation method (RMSEP = 0.44). As for hardness, the larger number of samples in this study might have contributed to larger RMSEP values. In addition, the correlation coefficient for the calibration model (R_c = 0.88, Table III) was higher than that reported by Meullenet et al (1999). However, with any of the architectures tested, the ANN models were not robust (RMSEP/RMSEC ≥ 1.65, Table II). This indicates that future prediction of this attribute for cooked rice may be inaccurate.

Roughness of mass was successfully predicted using ANN (RMSEP = 0.168 and 0.182, Table III). The models also discriminated highly between samples (S_{tot}/RMSEP = 6.03 and 6.53, Table III). In addition, in comparison to the model obtained using PLS regression, the RMSEP for ANN models were improved by 26% with a (7, 4, 2, 1) architecture and 19.8% with a (6, 4, 2, 1) and a (4, 3, 2, 1) architecture. However, the latter architecture yielded the most robust model (RMSEP/RMSEC = 1.05, Table III). A model with more input nodes (ANN [7, 4, 2, 1]) resulted in a lower RMSEP value (RMSEP = 0.168) and higher correlation for the prediction model (R_c = 0.90); however, the model (RMSEP/RMSEC = 1.28) was not as robust as models with lower number of input nodes (Table III). ANN improved the prediction of cooked rice toothpull. RMSEP values from all three architectures (RMSEP = 0.263, 0.277, and 0.269, Table III) were lower than the value from PLS regression (RMSEP = 0.356, Table II). However, the values from ANN were similar to that reported by Meullenet et al (1999) using PLS regression. RMSEP values from ANN were reduced most by 26.1% with a (7, 4, 2, 1) architecture. However, the number of input nodes in this architecture caused overfitting (RMSEP/RMSEC = 2.12, Table III). The most robust and discriminative model was obtained from a (4, 3, 2, 1) architecture (RMSEP/RMSEC = 1.14, RMSEP = 0.269, S_{tot}/RMSEP = 3.60, Table III). The ANN model with eight input nodes was somewhat robust (RMSEP/ RMSEC = 1.20, Table III); however, the RMSEP value (RMSEP = 0.277) was not as low as the value acquired from the previously discussed architecture. The increase in model robustness with a larger number of input nodes conflicts with other findings of this study. For other sensory attributes (hardness and adhesiveness to lips), models with a higher number of input nodes tended to cause overfitting. However, for toothpull, a (8, 4, 2, 1) architecture (RMSEP/RMSEC = 1.20, Table III) yielded a more robust than model with a (7, 4, 2, 1) architecture (RMSEP/RMSEC = 2.12, Table III). Hence, the differences observed in the ratio between RMSEP and RMSEC, an indication of model robustness, might not always be due to overfitting.

Prediction of particle size using two different ANN architectures was effective (RMSEP = 0.079 and 0.086, Table III). However, RMSEP values for ANN models were not largely decreased in comparison to the model obtained from PLS regression with the test set validation method (improvement of 13.2 and 5.5%, Table III). The most robust and discriminative model was obtained with a (2, 4, 2, 1) architecture (RMSEP/RMSEC = 1.11, S_{tot}/RMSEP = 3.70, Table III). As for most other attributes, a model with a higher number of input nodes (ANN [4, 3, 2, 1]) tended to be less robust (RMSEP/RMSEC = 1.30, Table III).

TABLE III
Models Statistic for Various Artificial Neural Network (ANN) Architectures

Sensory Attributes	Design[a]	Architecture	R_p[b]	RMSEP[c]	R_c[d]	RMSEC[e]	RMSEP/RMSEC	S_{tot}/RMSEP[f]	Improvement (%)[g]
Adhesiveness to lips	1	8, 4, 2, 1	0.88	0.463	0.94	0.337	1.37	3.83	21.3
	2	7, 4, 2, 1	0.89	0.445	0.89	0.445	1.00	3.99	24.3
	3	4, 3, 2, 1	0.88	0.456	0.88	0.476	0.96	3.89	22.5
Hardness	1	8, 4, 2, 1	0.87	0.331	0.95	0.175	1.89	2.35	7.8
	2	6, 4, 2, 1	0.88	0.315	0.96	0.155	2.03	2.47	12.3
	3	4, 3, 2, 1	0.87	0.326	0.84	0.299	1.09	2.39	10.9
Cohesiveness of mass (after 3 chews)	1	…	…	…	…	…	…	…	…
	2	2, 4, 2, 1	0.66	0.894	0.66	0.886	1.01	1.84	28.5
	3	4, 3, 2, 1	0.80	0.730	0.83	0.669	1.09	2.26	41.6
Cohesiveness of mass (after 8 chews)	1	5, 4, 2, 1	0.74	0.538	0.83	0.327	1.65	2.77	12.4
	2	4, 4, 2, 1	0.77	0.513	0.88	0.280	1.83	2.90	16.5
	3	4, 3, 2, 1	0.71	0.573	0.87	0.301	1.90	2.60	6.7
Roughness of mass	1	7, 4, 2, 1	0.90	0.168	0.91	0.131	1.28	6.53	26.0
	2	6, 4, 2, 1	0.87	0.182	0.86	0.160	1.14	6.03	19.8
	3	4, 3, 2, 1	0.87	0.182	0.83	0.174	1.05	6.03	19.8
Toothpull	1	7, 4, 2, 1	0.94	0.263	0.98	0.124	2.12	3.68	26.1
	2	8, 4, 2, 1	0.93	0.277	0.93	0.230	1.20	3.49	22.2
	3	4, 3, 2, 1	0.93	0.269	0.92	0.237	1.14	3.60	24.4
Particle size	1 and 2	2, 4, 2, 1	0.67	0.079	0.66	0.071	1.11	3.70	13.2
	3	4, 3, 2, 1	0.61	0.086	0.72	0.066	1.30	3.40	5.5
Toothpack	1	5, 4, 2, 1	0.84	0.340	0.96	0.137	2.48	2.70	22.4
	2	7, 4, 2, 1	0.82	0.350	0.98	0.109	3.21	2.62	20.1
	3	4, 3, 2, 1	0.82	0.342	0.94	0.163	2.10	2.68	21.9
Loose particles	1	8, 4, 2, 1	0.89	0.380	0.90	0.377	1.01	3.37	13.0
	2	7, 4, 2, 1	0.91	0.353	0.95	0.291	1.21	3.63	19.2
	3	4, 3, 2, 1	0.87	0.423	0.89	0.390	1.08	3.03	3.2

[a] Design 1: Number of input nodes equal to number of principal components (PC) suggested in partial least squares (PLS) regression (test set method); design 2: number of input nodes equal to number of PC suggested in PLS regression for full cross-validation; and design 3: number of input nodes = 4.
[b] Correlation for prediction model.
[c] Root mean square error of prediction.
[d] Correlation for calibration (training) model.
[e] Root mean square error of calibration.
[f] Standard deviation of a sensory attribute.
[g] Percent improvement = (RMSEP PLS [test set] – RMSEP ANN × 100)/RMSEP PLS (test set).

Toothpack was fairly well predicted using ANN (RMSEP = 0.340, 0.342 and 0.350, Table III) with RMSEP improvements between 20.1 and 22.4%. Although ANN models offered relatively low RMSEP values (RMSEP ≤ 0.35), the models exhibited a serious lack of robustness (RMSEP/RMSEC > 2.10). Models with higher number of input nodes had a tendency to be less robust. ANN also improved the prediction on the attribute loose particles with RMSEP values of 0.353–0.423 with three different networks (Table III). The RMSEP values reported here were somewhat larger than that reported by Meullenet et al (1999) (RMSEP = 0.22) using PLS regression. All ANN models were discriminated between samples satisfactorily (S_{tot}/RMSEP > 3). Models with a (8, 4, 2, 1) or a (7, 4, 2, 1) architecture yielded lower RMSEP values (RMSEP = 0.380 and 0.353, respectively, Table III) than the model evaluated with PLS regression with test set validation (RMSEP = 0.437, Table II). This represents an improvement of 13.0 and 19.2%, respectively. The model with a (4, 3, 2, 1) architecture (RMSEP = 0.423) provided the least improvement in terms of RMSEP value (3.2%). The most robust model was obtained from a (8, 4, 2, 1) architecture (RMSEP/RMSEC = 1.01).

CONCLUSIONS

ANN in combination with SSSA was successfully used to predict sensory texture profiles of cooked rice and was an effective modeling technique permitting the development of accurate instrumentation for predicting cooked rice texture. RMSEP values for all sensory attributes were lowered over PLS models when ANN was used. However, in some cases (toothpack), the ANN lacked robustness. Improvements offered by ANN models over PLS regression varied from attribute to attribute between 10.9 and 41.6%. In addition, the ratio between RMSEP and RMSEC, an indication of model robustness, were, as a general rule, closer to 1.0 when using ANN. The predictive models, even if not always dramatically improved, showed the potential of ANN as a modeling tool for predicting food texture from instrumental measurements. SSSA is a viable method for relating sensory perception of texture to instrumental data. Overall, ANN and SSSA used in combination, showed potential for developing as an "intelligent" system capable of predicting cooked rice texture profiles for most of the sensory attributes evaluated.

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