Neural Network Modeling of Physical Properties of Ground Wheat[1]

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ABSTRACT

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Physical properties of ground materials from roller mills are affected by the characteristics of wheat and the operational parameters of the roller mill. Backpropagation neural networks were designed, trained, and tested for the prediction of three physical properties of ground wheat: geometric mean diameter (GMD), specific surface area increase (SSAI), and break release (BR). Eight independent variables were used as input data. Compared to conventional statistical models, the accuracy of prediction was improved substantially, as reflected by the significant reduction in root mean squared error (RMS), relative error (RE), and the increase in coefficient of determination R^2 (>0.98). The neural network models are, therefore, capable of predicting the physical properties of the ground wheat.

Roller mills are widely used in flour mills to grind wheat into flour. A roller mill is adjusted so that ground materials with targeted physical properties are obtained. Physical properties of ground materials determine the final quality of the flour. The characteristics of the ground materials are affected by the properties of wheat as well as by the operational parameters of the roller mill (Fang et al 1995a).

The physical properties of wheat kernels include: class, cultivar, kernel hardness, kernel size, kernel weight, and moisture content. The operational parameters of a roller mill include: feed rate, fast roll speed, roll speed differential, and roll gap. Therefore, quality control of the physical properties of the ground material is a challenging task because so many variables are involved. On the other hand, automation of the roller mill requires the accurate prediction of physical properties of the ground materials according to the properties of the feedstock and the preset operational parameters of the roller mill.

Neural networks offer solutions to this kind of problem. Neural networks, a new class of information processing techniques, are offering solutions to problems that have not been explicitly formulated (Ruan et al 1995). Neural networks are finding more and more applications in the food industry. A backpropagation neural network was developed by Sayeed et al (1995) to predict the sensory attributes of a snack food. The performance of the trained neural network was reasonable. Liao et al (1993) used a neural network to classify corn kernel breakage. The neural network model accurately discriminated the broken kernels from the whole corn kernels. Ruan et al (1995) designed a neural network that accurately predicted (>94%) the rheological properties of dough from the torque developed during mixing. The authors claimed that the neural network could be used online for process control. Zhang et al (1992) presented a neural network model for prediction of the secondary structure of globular proteins. Based on knowledge of the secondary structure of the existing proteins, the model predicted the secondary structure of local sequences of amino acids with a success rate of 64.3%. Chen et al (1995) developed feedforward backpropagation neural networks to classify hard red winter wheats based on near-infrared reflectance (NIR) spectra data of ground wheat samples. The classification accuracies for hard red winter wheats of different crop years ranged from 95.1 to 97.0%.

As discussed previously, the physical properties of ground wheat are affected by multiple variables, and the analytical relationships between the physical properties and those variables involved have not been determined. Although statistical models have been examined (Fang 1995), neural network modeling may provide a better solution. Therefore, the objective of this study was to design and train neural networks capable of predicting three physical properties of roller-milled ground materials.

MATERIALS AND METHODS

Three different classes of wheat, soft red winter (SRW), hard red winter (HRW), and hard red spring (HRS), from the 1993 crop year were used to conduct milling experiments. The SRW wheat was grown in Ohio, the HRW wheat was grown in Kansas, and the HRS wheat was grown in North Dakota. The physical properties of these wheats are presented in Table I.

Fifty-four first-break milling tests were conducted using a computerized experimental roller mill (Fang et al 1995b). Six independent variables each at three levels, wheat class (SRW, HRW, and HRS), moisture content (14.5, 15.5, and 16.5% wb), feed rate (15, 20, and 25 kg/m·min), fast roll speed (425, 475, and 525 rev/min,), roll speed differential (3.1, 3.4, and 3.7 m/sec), and roll gap (0.66, 0.74, and 0.82 mm), were included in this study. A response surface experimental design was used.

The physical characteristics of the ground wheats, including geometric mean diameter (GMD), specific surface area increase (SSAI), and break release (BR), were determined using sieving methods. GMD is a measurement of the particle size based on the assumption that the ground wheat follows a log-normal particle-size distribution. SSAI measures the increase in surface area in a unit mass of ground stock, an indicator of grinding efficiency. GMD and SSAI were determined according to ASAE S319.1 (ASAE 1989). BR is a criterion used by millers to measure the particle size of the ground stock. BR was measured by sieving 100 g of ground stock on a 20W (1.0-mm opening) screen for 20 sec using a Great Western sifter. BR was calculated as the percentage of the ground stock passing through the 20W screen.

Neural Network Development

Individual neural networks were developed for GMD, SSAI, and BR. Fifty-four data points obtained from the milling tests were used for training and testing the neural networks. Ten percent of the total 54 data points (six data points) were reserved for testing the trained networks. BrainMaker Professional software (California Scientific Software, Nevada City, CA) was used in the neural network development. A total of eight input variables, moisture content (M), single kernel hardness index (H), single kernel size (S), single kernel weight (W), feed rate (F), fast roll speed (R), roll speed differential (D), and roll gap (G) were used. The single kernel properties of wheat were measured using the

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Single-Kernel Wheat Characterization System developed by the USDA Grain Marketing Research Center, Manhattan, KS (Martin et al 1993).

The root mean square error (RMS), relative error (RE), and coefficient of determination (R^2) were used as the criteria to evaluate the training process and the performance of the trained neural networks. The RMS was computed as the square root of the sum of squares of the differences between the network output data and the actual data divided by the number of facts. This way, larger errors are magnified. The RE was calculated as dividing the RMS by the mean of the actual data set.

When constructing a neural network, the number of hidden layers must be carefully chosen. In general, the fewer hidden layers, the better the network performs. As a starting point, all three neural networks were first trained with only one hidden layer. But, later we found that the neural network for GMD did not converge well during training. Therefore, two hidden layers were used for GMD.

The learning rate while training a network determines how large a correction should be made to the connection weights when it gets a fact wrong. An initially large learning rate will make the network learn the entire data set quickly. With the progress of training, the learning rate should be reduced gradually to fine-tune the network. The training processes started with an initial value of 1.0 for the learning rate and an initial value of 0.40 for the training tolerance, which means that the error of the output values must be within 40% of the original data to be considered correct. While training, both the learning rate and the tolerance were reduced gradually under the condition that >90% of the total facts have been correctly identified. At the final stages of training, the learning rate was set to “automatic” to let the networks converge by themselves. After each cycle of training, all networks were tested using the data set that the networks have never seen before. Based on the testing results, decisions were made to modify the network structure and training strategies.

To improve the robustness or the predictability of the trained neural networks, several techniques were used. First, the training data set was shuffled during training to randomize the sequences between data points. This way, information about the data set was randomly presented to the networks to avoid the networks “memorizing” a certain trend. Secondly, all trained networks were optimized using the Genetic Training Option (GTO) module (Version 3.11, California Scientific Software). The genetic algorithm is a methodology designed for searching a group of “best” solutions in a manner similar to the natural selection procedure in biological evolution.

TABLE I
Physical Properties of Wheat Samples

Physical Properties	Soft Red Winter	Hard Red Winter	Hard Red Spring
Bulk density (g/cm^3)	0.810	0.806	0.788
True density (g/cm^3)	1.368	1.414	1.396
1,000 kernel weight (g)	36.80	32.58	41.77
Single kernel hardness	9.06 ± 15.76	71.17 ± 17.2	68.83 ± 15.41
Single kernel weight (mg)	35.26 ± 6.98	31.56 ± 7.19	40.68 ± 8.45
Single kernel size (mm)	2.665 ± 0.36	2.556 ± 0.36	3.005 ± 0.46
Single kernel moisture (%, wb)	12.61 ± 0.24	12.69 ± 0.23	13.26 ±0.26
NIR hardness	23.0	50.3	86.0
Air oven moisture (%, wb)	12.54	12.41	13.15

TABLE II
Training Statistics[a] of the Three Neural Networks for Geometric Mean Diameter (GMD), Specific Surface Area Increase (SSAI), and Break Release (BR)

	GMD (mm)		SSAI (cm^2/g)		BR (%)	
LL/TT	RMS	R^2	RMS	R^2	RMS	R^2
1.0/0.10	0.0722	0.9167	0.0705	0.9260	0.0593	0.9355
1.0/0.08	0.0641	0.9336	0.0554	0.9552	· · ·	· · ·
1.0/0.06	0.0436	0.9654	· · ·	· · ·	0.0436	0.9649
0.8/0.06	· · ·[b]	· · ·	0.0382	0.9633	· · ·	· · ·
0.8/0.05	0.0381	0.9768	0.0352	0.9765	0.0309	0.9751
0.8/0.04	0.0305	0.9851	· · ·	· · ·	0.0345	0.9783
0.6/0.04	· · ·	· · ·	0.0292	0.9839	0.0254	0.9892
0.6/0.02	0.0109	0.9978	· · ·	· · ·	0.0222	0.9905
0.4/0.02	· · ·	· · ·	0.0277	0.987	0.0147	0.9956
Auto/0.02	0.0094	0.9982	0.022	0.9928	0.0143	0.9957

[a] LR/TT = learning rate/training tolerance. RMS = root mean square error; R^2 = coefficient of determination.

[b] LR/TT were not used.

TABLE III
Performance[a] of the Trained Neural Networks

	Output Variables		
Parameters[b]	GMD (mm)	SSAI (cm^2/g)	BR (%)
RMS	0.0071	1.1625	0.2311
RE (%)	0.57	2.60	1.04
R^2	0.991	0.987	0.986

[a] Geometric mean diameter (GMD), specific surface area increase (SSAI), and break release (BR).

[b] RMS = root mean square error; R^2 = coefficient of determination; RE = relative error.

RESULTS AND DISCUSSION

During training of the networks, two criteria, RMS and R^2, were used to monitor the training performance of the networks. The modifications during the training processes were done mainly according to the convergences of both RMS and R^2. Table II shows the major training statistics of the three networks for GMD, SSAI, and BR. For all three neural networks, the training processes converged well. The RMS values for GMD, SSAI, and BR were 0.0094, 0.022, and 0.0143, respectively. The R^2 values for all three models were >0.99.

During the network training process, the effects of the independent variables on the output variables were closely monitored. *H, S,* and *W* had significant positive effects on GMD. *F, R, D,* and *G* all had significant negative effects on GMD. The positive effects of *D* and *R* were significant on SSAI. *H, W,* and *G* had significant negative effects on SSAI. The positive effects of *M, F,* and *W* on BR were significant. *H* and *G* had significant negative effects on BR. The rest of the input variables had negligible effects on the corresponding response variables.

The overall performances of the three neural network models are summarized in Table III. All three networks performed well during testing. The network for GMD performed the best with an RMS of 0.007 and an RE of 0.57%. The network for BR had the second best testing statistics, with an RMS of 0.231 and an RE of 1.04%. The network for SSAI had the largest RMS of 1.162 and RE of 2.60%. All three networks also had R^2 values of ≈0.99, which indicated that the predicted values agreed well with the actual data points. The reason the GMD network had the best performance may have been due to the use of two hidden layers that were added later because the network with a single hidden layer of did not train well.

Previously, statistical models were constructed using a multiple linear regression technique to predict the physical properties of ground wheat materials (Fang 1995). Included in the study were six independent variables: single kernel hardness, moisture content, feed rate, fast roll speed, roll speed differential, and roll gap. The performances of the models were not as accurate as the neural network models.

Also, it is important to point out that a data set containing 54 data points was relatively small for training and testing a neural network. The limitation on available data points may hinder the prediction power of the developed neural network models. More data points are needed to further improve the neural network models. A separate and fairly large data set should be used to test the trained neural network models.

CONCLUSIONS

Three neural network models were developed to predict selected physical properties of the ground materials of wheat from first-break roller grinding. The selection of the numbers of hidden layers was critical to the design of the networks. Backpropagation networks converged well during training due to the correct choices of learning rates and training tolerances. The performances of the networks during testing were good. The accuracy of prediction was improved greatly over that of conventional statistical models.

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