OTM-BEEF RECOGNITION USING CHROMATOGRAPHIC DATA PROCESSED BY METALEARNING BASED CLASSIFIER

Erwin Oñate[1], Tomás Arredondo[2] and Cristian Acevedo[3]

1 Departamento de Electrónica, Universidad Técnica Federico Santa María, Valparaíso. Chile

2 Centro de Biotecnología, Universidad Técnica Federico Santa María, Valparaíso. Chile

Erwin.onate@alumnos.usm.cl

Abstract – In order to control bovine spongiform encephalopathy (BSE), a strategy called OTM was devised (thirty months). It requires the disposal of bovines older than thirty months from the food chain. Although bovine age can be estimated through dentition, this method cannot be applied to processed meat. Because of this, volatile organic compounds (VOCs) have been presently used for OTM (over thirty months) beef sample recognition. VOCs released by meat were sampled through gas chromatography. This was done from a set of more than 500 chromatograms (each one with 17 fully identified VOCs) of vacuum sealed, chilled and fresh meat. A classifier was developed using metalearning optimization methods and neural networks as the principal learner.

The optimized configuration of the neural network allowed it to discriminate between OTM and UTM (under thirty months) meat gathered from cattle, with a precision near 90%. The results were contrasted with traditional statistical methods like the linear discriminant analysis (LDA), soft independent modeling of class analogy (SIMCA), partial least squares discriminant analysis (PLS-DA) and support vector machine (SVM).

In conclusion, volatile organic compounds can be used for the recognition of bovine OTM meat in various presentations (fresh, chilled or vacuum sealed).

I. INTRODUCTION

Bovine spongiform encephalopathy (BSE) is a serious neurodegenerative disease affecting a significant number of the domestic cattle. This disease reached epidemic proportions in several European countries, as well as in Japan and North America [1]. There is also a variant of the Creutzfeldt- Jakob disease (vCJD) that is caused by the oral exposition to the BSE's agent [2]. With the purpose of controlling this disease, a strategy called OTM (over thirty months) was created. This strategy requires the disposal of bovines older than thirty months from the food chain. An OTM based regulation banned the sale of beef older than thirty months.

Processed meat, is difficult to label as OTM or UTM (under thirty months), because the animal's age can be best estimated by dentition (the processed meat does not have teeth). This situation is a common classification problem, where adequate information can be used for the training of mathematical algorithms and generates decision rules. Previous works have informed that the age of mammals could be correlated with their volatile profile [3] and the volatile organic compounds (VOC) can be used to discriminate between OTM and UTM [4]. Artificial neural networks (ANN) have been successfully used as a tool for the modeling and study of complex problems in the area of biology and biochemistry [5, 6, 7, 8].

Previous investigations have used the information generated by gas chromatography (GC/MS) for development of high precision classifiers for the recognition and discrimination of UTM and OTM [4]. In this present work, we have extended this investigation with fresh meat, chilled meat and vacuum sealed meat and a complete characterization of the bovine meat volatile release profile considering 17 VOCs. The information of more than 500 volatile profiles was used for the development of a binary sorter for the discrimination between OTM and UTM using ANN.

II. MATERIALS AND METHODS

1. *Samples*

The meat samples were obtained from *M. longissimus dorsi* Holstein (*Bos taurus*). In the analyzed samples there are male and female cattle with 5 different dentitions (0, 2, 4, 6 and 8 definitive incisive teeth). More of 500 samples are sorted for 7 types of meat: fresh meat, chilled meat for 3, 5 and 7 days; and vacuum sealed meat for 15, 30 and 60 days. A total of 525 chromatograms (one for each sample) were obtained which were considered as OTM if the sample came from a bovine with 2 or more definitive incisive teeth [9].

2. *Volatile organic compounds*

We analyzed the release of volatile molecules from beef by means of a GC/MS-SPME (Gas chromatography / mass spectrum - Solid phase micro extraction). We used the method described previously by [4].
Potential emanations were analyzed by using the Finnigan Xcalibur Software (Thermo Electron Corporation) matching mass spectrums with those saved in the NIST MS Spectral Library 2008. Selected chromatographic peaks were checked with their respective chemical standards and retention indexes.

3. *Classification*

A binary sorting was made (classes labeled as UTM or OTM) through the use of chromatographic profiles by using ANN. This was contrasted with other methods such as the linear discriminant analysis (LDA), soft independent modeling of class analogy (SIMCA), partial least squares discriminant analysis (PLS-DA) and support vector machine (SVM). The SIMCA and PLS-DA calculations were made using the SIMCA-P software (Umetrics) and for SVM the LibSVM software was used with a gaussian kernel [10].
For the entire set of data (525 chromatograms), we applied random sampling with cross validation [11] toward the generation of training sets and tests in a 50/50 proportion. This selection was repeated thirty times using a uniformly distributed random selection procedure. This gives rise to thirty different data sets used for the classification (by each one of the methods previously indicated).

4. *Neural Network*

The neural network used, is a feed forward artificial neural network (FFANN). This network is constituted by three layers including a hidden layer. With a multilayer neural network like this one, it is possible to model highly nonlinear decision surfaces. This is a requirement for complex classification problems [12].
Our FFANN was trained with the backpropagation algorithm [13, 14], due to its general simplicity and good performance in a variety of classification and modeling of difficult problems [15]. The input layer is composed of 17 neurons, one for each volatile organic compound (VOC). In basic neural network configuration, the amount neurons in the hidden layer are adjusted through a manual iterative process. The basic neural network configuration (before optimization) is used as a basic classifier. In the output layer there is only one neuron taking in account that we are interested in only one class (OTM or UTM). In our implementation of a basic FFANN, the learning rate and the impulse were fixed with a floor of 0.01 for each, this was a reasonable empirically obtained value [16]. A maximum of 2.5 million iteration were used for the training algorithm after an ad-hoc experimental process that was performed toward the determination of a reasonable number of iterations in this problem context.

5. *Neural network based metalearning*

Meta-learning is a machine learning methodology where the learning algorithms are applied to the metadata related with an automatic learning process. The main goal of meta-learning is to improve the performance of existing learning algorithms. In the literature there are different definitions available of what is “meta-learning”. In [17] meta-learning is defined as the capacity of changing a learner with the objective of achieving a better performance. In [18] meta-learning is defined as learning algorithms that improve their dynamic tendency through the experience of the accumulation of meta-knowledge. In our approach, we have optimized the neural network described before, adjusting the number of neurons in the hidden layer, the learning rate and the momentum using genetic algorithms (GA). The fitness function used is the neural network’s classification success rate. The meta-learning process (namely a GA) tries to determine which is the best parameter vector with the goal of finding the best configuration for the neural network.

III. RESULTS AND DISCUSSION

An exploratory analysis of the chromatography data took place by using a simple LDA [19]. The average precision was close to 67 %. This preliminary analysis indicated the presence of a complex data distribution and the impossibility to use a simple classification procedure for the discrimination between UTM and OTM.
The strategy used in [4] allows an excellent discrimination between UTM and OTM meat using a PLS-DA and SIMCA based parallel classifier [20]. This classifier was more precise

than SVM [21]. However, only fresh meat was tested. In this present work, we have extended the investigation with three bovine meat types (fresh meat, chilled meat and vacuum sealed meat). The results obtained with LDA, PLS-DA, SIMCA and SVM are informed in Table 1. The obtained results with the methods mentioned before weren't enough to get a satisfactory discrimination between UTM and OTM meats. This motived our investigation about the use of neural networks (ANN) that were optimized by meta-learning.

Table 1. Accuracy for all classifiers evaluated on the test-set.

	Average	Minimum	Maximum
LDA	67.3 (±1.69)	65.0	70.7
SIMCA	63.5 (±2.77)	56.4	69.2
PLS-DA	66.4 (±1.71)	63.5	69.9
SVM	76.6 (±1.91)	73.4	79.9
FFANN	81.9 (±2.10)	78.4	87.6
OML-NN	84.3(±1.74)	81.1	89.2

LDA: Linear Discriminant Analysis; SIMCA: Soft Independent Modeling of Class Analogy; PLS-DA: Partial Least Squares Discriminant Analysis; SVM: Support Vector Machine; FFANN: Feed Forward Artificial Neural Network; OML-NN: Optimal Meta Learner

The precision of the ANN was significantly higher than SVM (see Table 1). However, with an average precision close to 82%, the FFANN was still low for using as an appropriate classifier.

In our present optimization approach, we used the meta-learning process described before with the purpose of generating thirty optimal configurations for the learner (neural network).

Starting from the obtained 30 optimal configurations 30 neural networks were trained (with each training/test pair) for every Meta-learner configuration. From these meta-learners we can select the most adequate for each data set; these are labeled as Optimal Meta Learner (OML-NN). The best results of the OML configuration in an approximate precision of 90 % (see table 1).

In every used data set the accuracy of OML-NN was better than FFANN, which indicates that in the 100% of the cases the accuracy of the OML-NN was significantly higher than FFANN.

IV. CONCLUSION

In conclusion, the volatile organic compounds can be used for the recognition of bovine OTM meat in any presentation (fresh, chilled or vacuum sealed meat).

The best configuration for OTM meat recognition sorters is OML-NN, with a precision near to 90%. As can be seen in Table 1, it was a significantly better result compared with other sorting methods.

The meta-learner optimized neural network allows to develop a more accurate sorter than others methods, including LDA, SIMCA, PLS-DA, SVM and basic FFANN. These sorting methods are well known and widely used with success in a variety of classifiers but for the problem at hand, they have failed to reach a good precision, even after careful manual tuning process. This speaks of the inherent difficulty present in the classification problem that may be due to the data's multidimensional complexity at hand. To the best of our knowledge, our current approach based in the optimization of chromatographic neural networks is the first to address the important issue of the food safety in relation to meat. This application could be of benefit to industry as well as regulators in order to assist traceability systems currently in place.

ACKNOWLEDGEMENTS

This research was partially funded by the DGIP of UTFSM (231356) and by FONDEF Grant D08i1102.

REFERENCES

1. Adkin, A., Webster, V., Arnold, M., Wells, G., and Matthews, D. (2010) Estimating the impact on the food chain of changing bovine spongiform encephalopathy (BSE) control measures: the BSE control model. Preventive Veterinary Medicine, 93(2–3), 170–182.
2. Acevedo, C.A., Sánchez, E., Reyes, J. and Young, M.E. (2010) Volatile profiles of human skin cell cultures in different degrees of senescence. Journal of Chromatography B, 878(3), 449-455.
3. Bouckaert, R. R. and Frank, E., (2004) Evaluating the Replicability of Significance Tests for Comparing Learning Algorithms. Lecture Notes in Computer Science, (3056), 3-12.
4. Santander R., Creixell W., Sánchez E., Tomic G., Silva J. and Acevedo C. (2013) Recognizing Age at Slaughter of Cattle from Beef Samples Using GC/MS–SPME Chromatographic Method. In Food Bioprocess Technology.

5. Arredondo, T., Oñate, E., Santander, R., Tomic, G., Silva, J. R., Sánchez, E., & Acevedo, C. A. (2014). Application of Neural Networks and Meta-Learners to Recognize Beef from OTM Cattle by Using Volatile Organic Compounds. *Food and Bioprocess Technology*, 1-9.(In Press)
6. Hill, B. D., Jones, S. D. M., Robertson, W. M., & Major, I. T. (2000). Neural network modeling of carcass measurements to predict beef tenderness.*Canadian Journal of Animal Science*, *80*(2), 311-318.
7. Panigrahi, S., Balasubramanian, S., Gu, H., Logue, C., & Marchello, M. (2006). Neural-network-integrated electronic nose system for identification of spoiled beef. *LWT-Food Science and Technology*, *39*(2), 135-145.
8. Park, B., Chen, Y. R., Whittaker, A. D., Miller, R. K., & Hale, D. S. (1994). Neural network modeling for beef sensory evaluation. *Transactions of the ASAE*, *37*(5), 1547-1553.
9. European Commission (2009). Commission Regulation (EC) No 620/ 2009 of 13 July 2009 providing for the administration of an import tariff quota for high-quality beef.
10. Chang, C. C., & Lin, C. J. (2011). LIBSVM: a library for support vector machines. *ACM Transactions on Intelligent Systems and Technology (TIST)*,*2*(3), 27.
11. Bouckaert, R. R. and Frank, E., (2004) Evaluating the Replicability of Significance Tests for Comparing Learning Algorithms. Lecture Notes in Computer Science, (3056), 3-12.
12. Mitchell, T., (1997) *Machine Learning* (1 ed.). McGraw-Hill, Inc., New York, NY, USA.
13. Werbos, P., (1974) Beyond Regression: New Tools for Prediction and Analysis in the Behavioral Sciences. PhD diss., Harvard University.
14. Hecht-Nielsen. (1989) Theory of the backpropagation neural network. In *Neural networks for perception (Vol. 1)*, Harry Wechsler (Ed.). Harcourt Brace & Co., Orlando, FL, USA 65-93.
15. Neelakanta, P.S., (1994) Information Theoretic Aspects of Neural Networks. Taylor & Francis Group, Florida, USA.
16. Leiva, M., Arredondo, T.V., Candel, D., Dombrovskaia, L., Agulló, L., Seeger, M., and Vásquez, F., (2009) Feed-forward Artificial Neural Network based inference system applied in bioinformatics data-mining. In: International Joint Conference on Neural Networks, Atlanta, pp. 1744-1749.
17. Haykin S., (1983). "Why should machines learn?" in Machine Learning: An Artificial Intelligence Approach, R. Michalski, J. Carbonnel, and T. Mitchell, Eds. Palo Alto, CA: Tioga, pp. 25–37.
18. Vilalta, R., and Drissi, Y., (2002) A perspective view and survey of meta-learning. *Artif. Intell.* 18(2), 77-95.
19. Martínez, A. M. and Kak, A. C., (2001). PCA versus LDA. *IEEE Trans. Pattern Anal,* 23(2), 228-233.
20. LIU, L. and Ã–ZSU, M.T., (2010) Handbook of Partial Least. Squares Springer Handbooks of Computational Statistics, pp 757-774.
21. Vapnik, V., (1995). *The Nature of Statistical Learning Theory*, Springer-Verlag.