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**Connectionist Methods for Classification of Fruit
Populations Based On Visible-Near Infrared
Spectrophotometry Data**

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Connectionist Methods for Classification of Fruit Populations Based On Visible-Near Infrared Spectrophotometry Data

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Abstract

Variation in fruit maturation can influence harvest timing and duration, post-harvest fruit attributes and consumer acceptability. Present methods of managing and identifying lines of fruit with specific attributes both in commercial fruit production systems and breeding programs are limited by a lack of suitable tools to characterise fruit attributes at different stages of development in order to predict fruit behaviour at harvest, during storage or in relation to consumer acceptance. With visible-near infrared (VNIR) reflectance spectroscopy a vast array of analytical information is collected rapidly with a minimum of sample pre-treatment. VNIR spectra contain information about the amount and the composition of constituents within fruit. This information can be obtained from intact fruit at different stage of development. Spectroscopic data is processed using chemometrics techniques such as principal component analysis (PCA), discriminant analysis and/or connectionist approaches in order to extract qualitative and quantitative information for classification and predictive purposes. In this paper, we will illustrate the effectiveness of a model, connectionist and hybrid approaches, for fruit quality classification problems.

1 Introduction

Variations in fruit development can affect fruit composition, maturity, storage attributes and sensory properties. Visible-near infrared (VNIR) reflectance spectroscopy collects a

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large volume of data rapidly and non-destructively at any stage of development. Hence, visible-near infrared (VNIR) spectroscopy is widely used for monitoring the composition and quality of agricultural and pharmaceutical products, and food industry.

Over the last few years the number of papers devoted to connectionist approaches has increased significantly in the field of near infrared (NIR) reflectance and transmittance spectroscopy. Artificial neural networks (ANNs) have been used to find non-linear relationships between NIR reflectance and transmittance spectral data and analyte concentration ([15, 21, 5, 3]). Most of these efforts have been focused on determining whether connectionist approaches could improve upon the traditional calibration methods such as stepwise regression, principal component regression (PCR) and partial least squares (PLS).

Furthermore, while ANNs have been used for quantitative NIR analysis, a limited amount of work has been carried out on their use for NIR qualitative measurement and hybrid approaches between neural networks (NNs) and fuzzy logic theory. The synergism of integrating neural networks and fuzzy logic systems [22] into a functional system provides a new direction towards the realization of intelligent systems [14], [7], and [8].

VNIR diffuse body reflectance spectra have been used to characterise fruit during ripening at different stage of development [16, 17]. The aim of the present work was to investigate the use of full VNIR spectra sampled over the 500–1000nm to discriminate between kiwifruit managed to resemble extremes in fruit quality and compositional variation that might be encountered in practice, and to predict at the time of harvest, the ultimate soluble solids and dry matter content after full ripening, and the occurrence of storage disorders. In order to tackle these problems of the NIR spectra from kiwifruit, we illustrated two problems and investigated such various techniques as statistical based discriminant approach, supervised neural network learning methods, and a hybrid fuzzy neural network.

Firstly, the NIR spectra from kiwifruit was obtained from the 4 different cane treatments (*Control*, *Ethephone*, *Foil shade*, and *Leaf removal*) during the different stages of development for fruit quality and compositional classification problem. That is, in ripened kiwifruit (*Actinidia Deliciosa* ‘Hayward’), VNIR spectra can reveal information about treatments applied before harvest and after storage even though the compositional differences were small [17, 11].

Secondly, this paper also illustrates the use of these techniques to characterise changes in kiwifruit during storage and ripening, and at harvest, i.e., to classify the ripeness stages for the spectra. We are interested in being able to predict each fruit originally identified by spectra collected at harvest from spectra collected after storage or after ripening. As the spectra change after storage and ripening, these changes may be predictable. In this case, the same fruit have been measured at the 3 intervals (at harvest, after storage, after ripening), in which the spectra are the *ethephone treatment*.

In this paper we describe data collection and analysis in section 2. In section 3 a brief description of neural networks are introduced, and the use of cross validation and the training procedure are explained. Application examples and experimental results in two classification problems mentioned in the previous paragraphs: treated kiwifruit and kiwifruit at different ripening stages are given in section 4. Section 5 concludes this paper by giving succinct summary and future directions of this work.

2 Data collection and Feature Selection

2.1 Data Collection and Preprocessing

Diffuse body reflectance VNIR spectra are sensitive to the fruit structural, textural and compositional changes associated with pre-harvest influences on fruit quality and composition. Diffuse body reflectance VNIR spectra (540–1000nm range sampled at about 0.5nm) were collected from the equator of intact fruit using a portable miniature fibre optic probe and charged couple device spectrophotometer (PS1, Ocean Optics Inc., Florida). Grams 32 software (Galatic Industries, Salem, NH) was used to pre-process the raw spectra. The raw sample and reference spectra were processed by a Savitsky–Golay convolution smoothing algorithms (second order polynomial at ten intervals), and the absorption spectra were calculated ($\text{Log}(\text{reference/sample})$). The derivatisation removed any baseline and linear shifts in the spectra [2].

In the first case, Kiwifruit (*Actinidia deliciosa* ‘Hayward’) vines were manipulated by removing leaves, by shading the fruit in aluminium foil, or by spraying the fruit with ethephon (7 mg/L) during the developmental phase. Variation in fruit properties at harvest or after storage have been induced in fruit species (kiwifruit) by applying manipulation treatments to populations of fruit within a tree during pre-harvest development. The four treatments were control, plucked leaves, fruit wrapped loosely in aluminium foil to exclude light, and fruit sprayed ca 70 days after full bloom with ethrel. For each of the 4 treatments for the sampling date of 143 days (prior to storage) 150 individual fruit spectra collected against 873 wavelengths (data points), i.e., spectra were collected from 150 fruits per treatment at the time of harvest and again after the fruit had been stored for 16 weeks at 0°C and data was truncated to a 545–995nm range and a second order derivative calculated with a 10nm gap, giving a data set of 873 values for each fruit and sampling time.

In the second problem, kiwifruit were sprayed with *ethephone* (7 mg/L) 2 weeks prior to harvest to advance and synchronise maturation. After harvest, 150 fruit were stored for 16 weeks at 0°C and then allowed to ripen at ambient for 2 weeks. VNIR spectra of the equatorial region were recorded using a fibre optic probe at harvest, after storage, and again after ripening for each fruit. The each raw absorption spectra on the ripeness stages contains 150 spectra with 957 data points, representing the whole of the sample spectra.

The Figures 1 and 2 presented on this section illustrate the NIR spectra of a large number of substances of kiwifruit samples for the first case at harvest and for the second case, respectively.

2.2 Feature Selection

Using all data points in a spectra as inputs is a major problem in this study. There needs to be a data reduction step. Using the intensities of the mass spectra directly as input data vectors for the various methods under test showed to be not manageable because of the large dimensionality of the input data space. This problem is called the curse of dimensionality.

In order to give reasonable training times and to have data sets of comparable size only small subsets of each class of problems need to be selected. The reduction and transformation of the input data space by introducing spectral features can greatly enhance the performance of classification. The approach adopted was to reduce and transform the input data space by using well-established techniques based on principal component analysis (PCA), i.e., the

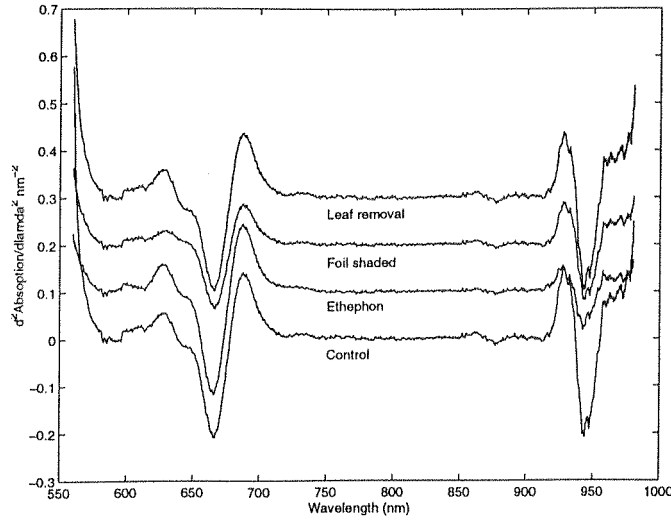


Figure 1: Visible-near infrared absorption spectra for kiwifruit at harvest.

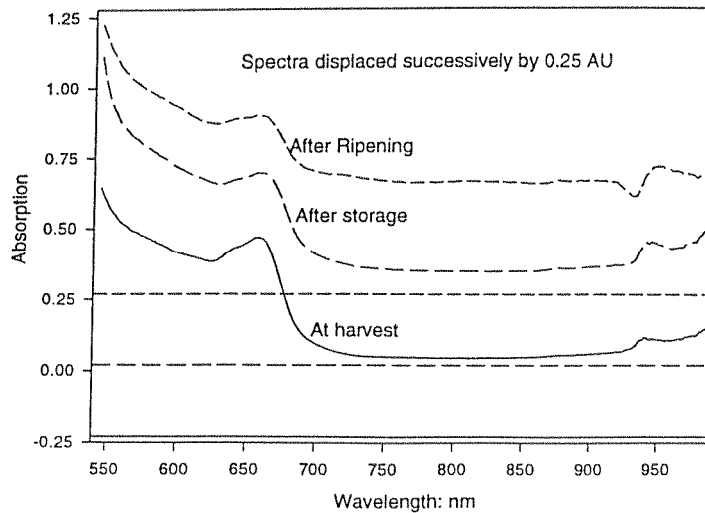


Figure 2: Visible-near infrared absorption spectra for stored kiwifruit.

raw absorption spectra were reduced to weighted sums of principle component (PC) spectra, derived from the spectra of all the fruit at all times.

In this way the size of each fruit data set was reduced to a much smaller number of factors scores which were then used to discriminate the treatments and categorise temporal changes. Training sets consisted of 75 spectra from individual fruit per treatment and time and the remaining fruit 75 spectra were then used for the validation sets in both chemometrics and hybrid connectionist approaches. In particular, the presence of a bimodal distribution in the foil treatment was previously determined and was included in the validation but not in the training set, in order to test the performance of classification under conditions where primary features are influenced by secondary factors. The validation spectra were projected onto the principal components (eigenvectors) derived from the training sets, thus reducing the size of each fruit data set to a much smaller number of factors scores.

In the first case, the size of each fruit data set was reduced to 13 factors for spectra at harvest and 21 factors after storage which were then used to discriminate the treatments.

In the second case, a satisfactory experiment was achieved by using the first 8 PCs. The extent that the PC weightings were characteristic of the ripeness stage was investigated by canonical discrimination using the spectra for 75 randomly selected fruit as a training set. The resulting algorithm was used to classify the ripeness stage for the spectra from the remaining fruit, validation set.

3 Methodology of Connectionist Approaches

3.1 Connectionist Approaches

The fuzzy neural network FuNN [8, 9, 10] uses a multi-layered perceptron (MLP) network and an extended BP training algorithm. In this connectionist structure, the input and output nodes represent the input states and output control/decision signals respectively, and in the hidden layers, there are nodes functioning as membership functions (MFs) and rules. This eliminates the disadvantage of a normal feedforward multi-layer net which is difficult for an outside observer to understand or to modify.

The architecture facilitates learning from data and approximate reasoning, as well as fuzzy rule extraction and insertion. It allows for the combination of both numerical and fuzzy data and fuzzy rules to be used in one system, thus producing the synergistic benefits associated with the two sources. In addition, it allows for adaptive learning in a dynamically changing environment.

The general FuNN architecture consists of 5 layers with partial feedforward connections as shown in Fig. 3. In this connectionist structure a modified BP training algorithm was developed. Nodes in layer one are input nodes which represent input linguistic variables [23] and the first and last layer act as the fuzzifier and the defuzzifier, respectively. In the condition layer, uniformly distributed triangular membership functions are used. Singletons are applied in between the action and the output layer, as connection weights, which represent the centre of a membership functions. FuNN is also adaptable where the membership functions of the fuzzy predicates, as well as the fuzzy rules inserted before training or adaptation, may adapt and change according to new training data.

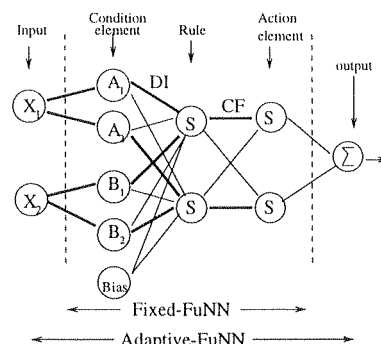


Figure 3: A FuNN structure for two input variables with two linguistic labels

For details of the supervised learning algorithms of FuNN, see [10].

Table 1: Classification Results at Harvest for the FuNN

Treatments	Control	Ethephon	Foil	Leaf
Control	73	0	0	0
Ethephon	1	73	2	0
Foil shade	0	2	73	1
Leaf removal	1	0	0	74
% misclassified	2.7	2.7	2.7	1.3

4 Application Examples

4.1 Results In Application To Treated Kiwifruit

Fig. 3 shows a structural outline of the FuNN that was selected for use in this study. The number of input and output nodes were fixed at 13 and 4 at harvest and 21 and 4 after storage model, respectively, but between 2 and 5 fuzzy subspaces were tested for input and output linguistic variables, and from 5 and 15 nodes of the rule layer were trained. The sigmoid activation functions for the rule and action layer were used, and the momentum terms were also implemented in order to accelerate the learning process. When training the MLP, the opportunity arose for selecting two adjustable learning parameters, the learning rate (η) and the momentum factor (α). FuNN has a speed up mechanism that adjusts these two parameters dynamically. This mechanism introduced two new variables, an upper bound and an increasing rate for η and α . These were calculated from the variations in the sum-squared error (SSE) measure after each epoch, as this gave an indication of how the weights changed.

For this study, the network was initialised with small random weights, which were scaled to unit variance before the scores were fed to the networks. Five rules in the rule layer at harvest model and ten rules after storage model and three membership functions associated with each input and output linguistic variables were finally selected for our discussion. After the training process had been iterated 2000 times, the convergence of the error (RMSE) decreased to 0.00188 at harvest and to 0.0883 after storage. The resulting models were tested on the validation sets which were not used in the training phase. Table 1 and 2 show the results of the classification by the FuNN of each model.

4.1.1 Example 1: At Harvest

In FuNN environment, we have constructed a model which is functionally equivalent to a *Generalisation Production rule* type of fuzzy inference system [8, p. 192]. Five fuzzy if-then rules (fruit at harvest) of the type from FuNN were extracted:

1. **if** <I7 is C 12.8> and <I10 is C 11.6> and <I11 is A 16.2> and <I12 is A 14.4> and <I13 is A 14.5> **then** <O1 is B 13.5> and <O2 is C 1.0> and <O3 is B 2.8> and <O4 is C 12.6>;
2. **if** <I11 is C 10.5> and <I12 is B 11.5> and <I13 is C 12.2> **then** <O1 is C 7.3> and <O2 is B 1.3> and <O3 is B 10.1> and <O4 is B 5.7>;

Table 2: Classification Results after Storage for the FuNN

Treatments	Control	Ethephon	Foil	Leaf
Control	53	0	0	3
Ethephon	1	75	1	0
Foil shade	0	0	74	0
Leaf removal	21	0	0	72
% misclassified	29.3	0	1.3	4.0

3. **if** <I12 is A 12.2> and <I13 is A 11.5> **then** <O1 is B 3.5> and <O2 is C 12.2> and <O3 is C 4.5> and <O4 is B 17.9>;
4. **if** <I6 is C 10.5> **then** <O1 is C 0.7> and <O2 is B 12.4> and <O3 is C 13.3> and <O4 is B 2.2>;
5. **if** <I13 is A 1.6> **then** <O1 is C 0.4> and <O2 is B 6.9> and <O3 is B 8.0> and <O4 is B 1.3>,

where I and O represent input and output variables, respectively, and A, B, and C denote fuzzy subspaces like small, medium, and large.

4.1.2 Example 2: After Storage

Ten fuzzy if-then rules of the same type for fruit after storage were also extracted from FuNN:

1. **if** <I2 is B 1.6> and <I17 is B 1.9> and <I21 is B 1.7> **then** <O2 is B 1.5> and <O3 is B 2.0> and <O4 is B 2.8>;
2. **if** <I8 is B 10.9> and <I11 is B 5.2> and <I15 is B 7.0> and <I17 is A 5.4> and **then** <O1 is B 5.0>;
3. **if** <I1 is B 2.7> and <I4 is B 2.2> and <I5 is C 2.1> and <I17 is A 3.2> and <I21 is B 2.0> **then** <O1 is C 2.7> and <O4 is B 2.5>;
4. **if** <I1 is B 7.7> and <I5 is C 5.9> and <I21 is A 6.6> **then** <O1 is B 6.4> and <O4 is C 6.6>;
5. **if** <I1 is B 14.3> and <I5 is A 8.1> and <I6 is A 5.2> and <I7 is A 9.0> and <I8 is B 10.7> and <I13 is A 10.1> and <I15 is B 20.1> and <I17 is B 29.4> and <I18 is A 7.3> and <I19 is A 7.8> and <I20 is C 7.2> and <I21 is A 30.5> **then** <O1 is B 4.2> and <O4 is C 4.1>;
6. **if** <I10 is A 6.0> and <I15 is B 5.3> and <I21 is A 11.2> **then** <O1 is B 1.1> and <O3 is C 4.5> and <O4 is B 3.4>;
7. **if** <I17 is B 9.1> and <I21 is A 10.6> **then** <O2 is C 4.5> and <O3 is B 4.5>;
8. **if** <I8 is B 7.7> and <I9 is C 6.5> and <I17 is B 7.2> **then** <O1 is C 0.8> and <O2 is B 0.7> and <O4 is C 0.7>;

Table 3: Classification Results at different Ripening Stages for the FuNN

Ripening Stages	At harvest	After storage	After ripening
At harvest	71	0	0
After storage	4	75	0
After ripening	0	0	75
% misclassified	5.33	0	0

9. **if** <I5 is C 4.3> and <I7 is B 4.6> and <I11 is C 8.1> and <I17 is A 11.1> and <I21 is B 6.5> **then** <O1 is C 4.5> and <O4 is B 4.2>;
10. **if** <I7 is C 6.5> and <I8 is C 8.7> and <I9 is B 8.0> and <I13 is B 6.3> and <I15 is A 5.0> and <I17 is A 9.0> **then** <O1 is C 3.6> and <O2 is B 3.5> and <O4 is B 3.0>,

where I and O also represent input and output variables, respectively, and A, B, and C denote fuzzy subspaces like small, medium, and large. It should be noted that the coefficients after each fuzzy predicate denote the degree of importance (DI) and confidence factor (CF) [8].

4.2 Results In Application To Kiwifruit At Different Ripening Stages

In this experiment, the number of input and output nodes were fixed at 8 and 3, respectively, but 3 triangular membership functions were tested for input and output linguistic variables, and 11 nodes of the rule layer were trained. The network was also initialised with small random weights, which were scaled to unit variance before the scores were fed to the networks. 11 rules in the rule layer for the model and three membership functions associated with each input and output linguistic variables were finally selected for the experiment. After the training process had been iterated 5000 times, the convergence of the error (RMSE) decreased to 0.005. The resulting models were tested on the validation sets which were not used in the training phase.

4.2.1 Example 3: Different Ripening Stages

Table 3 shows the results of the classification by the FuNN and 11 fuzzy if-then rules of the same type for different ripening stages were extracted:

1. **if** <I1 is B 4.9> and <I2 is C 15.6> and <I3 is C 4.4> and <I4 is B 4.8> and <I5 is A 3.5> and <I6 is C 8.7> and <I7 is A 3.9> and <I8 is A 2.1> **then** <O1 is C 2.7> and <O3 is A 1.5>;
2. **if** <I1 is B 1.9> and <I2 is B 7.0> and <I3 is A 1.95> and <I4 is A 3.3> and <I5 is B 1.2> and <I6 is C 3.0> and <I7 is A 0.2> and <I8 is A 2.4> **then** <O1 is C 1.0> and <O2 is A 2.7> and <O3 is A 0.3>;
3. **if** <I1 is B 14.5> and <I2 is B 1.7> and <I3 is C 5.9> and <I4 is A 5.9> and <I5 is B 12.5> and <I7 is A 5.2> **then** <O1 is B 0.004> and <O2 is B 0.004> and <O3 is B 0.004>;

4. **if** <I1 is C 3.0> and <I2 is A 5.7> and <I3 is A 1.3> and <I4 is A 4.6> and <I5 is C 3.7> and <I6 is B 4.4> and <I7 is B 3.1> and <I8 is A 1.8> **then** <O2 is A 0.3>;
5. **if** <I1 is C 32.4> and <I2 is C 8.3> and <I3 is C 11.5> and <I4 is A 30.7> and <I5 is C 8.7> and <I6 is B 9.9> and <I7 is B 14.2> and <I8 is A 9.0> **then** <O1 is A 2.6> and <O2 is C 7.1> and <O3 is B 0.03>;
6. **if** <I1 is B 8.2> and <I2 is A 16.2> and <I3 is B 1.1> and <I4 is C 0.6> and <I5 is C 0.6> and <I6 is A 9.5> and <I7 is B 1.4> **then** <O1 is A 2.8> and <O2 is C 0.4> and <O3 is B 0.03>;
7. **if** <I1 is A 1.4> and <I2 is C 1.7> and <I3 is A 7.8> and <I4 is B 18.2> and <I5 is C 5.2> and <I6 is C 12.3> and <I7 is A 3.4> **then** <O1 is A 5.1> and <O2 is C 5.98>;
8. **if** <I1 is B 12.8> and <I2 is B 11.8> and <I3 is B 9.95> and <I4 is B 6.9> and <I5 is C 1.1> and <I6 is A 7.4> and <I7 is A 6.1> and <I8 is C 10.03> **then** <O1 is B 0.03> and <O2 is A 3.04> and <O3 is C 0.13>;
9. **if** <I1 is C 13.3> and <I2 is A 4.1> and <I3 is A 7.3> and <I4 is A 2.4> and <I5 is C 3.5> and <I6 is C 3.4> and <I7 is B 1.3> and <I8 is A 3.3> **then** <O1 is B 0.05> and <O2 is A 2.6> and <O3 is A 0.2>;
10. **if** <I1 is B 1.2> and <I2 is A 4.2> and <I3 is A 0.7> and <I4 is A 0.9> and <I5 is C 1.04> and <I6 is A 0.5> and <I7 is A 0.4> and <I8 is A 1.7> **then** <O1 is A 1.6> and <O2 is A 2.5> and <O3 is C 3.04>;
11. **if** <I1 is A 2.7> and <I2 is A 12.9> and <I3 is A 2.8> and <I4 is A 6.1> and <I5 is C 5.7> and <I6 is A 4.5> and <I7 is B 2.4> and <I8 is B 1.2> **then** <O1 is A 1.4> and <O2 is A 1.2> and <O3 is C 1.4>.

5 Conclusion and Future Directions

Both statistically based methods (e.g. principal component (PC) and linear discrimination analysis), and artificial neural networks (ANNs) have been used to find relationships between NIR reflectance and transmittance spectral data for multivariate quantification of physical properties and for qualitative classification. The majority of work has been done using the statistical approach, and the efforts with ANNs have focused on determining whether such connectionist approaches could improve upon the traditional calibration methods, particularly in systems where substantial non-linearity is expected [2].

In this study, spectroscopic data was processed by using a hybrid fuzzy neural approach. Using the spectra from kiwifruit treated during the preharvest development and kiwifruit at the different ripening stages, the classification performance of the fuzzy neural network (FuNN) approach was demonstrated for each problem.

Neural networks give to fuzzy logic systems fault tolerance, distributed representation properties, and the learning abilities, while fuzzy logic systems provide a structural framework with high-level fuzzy *if-then* rules thinking and reasoning to the neural networks. In

general this synergism is complementary rather than competitive. For this reason, it is frequently advantageous to use neural networks and fuzzy logic in combination rather than exclusively, leading to so-called hybrid intelligent systems. They share the common ability to improve the intelligence of the systems working in an uncertain, imprecise and noisy environment.

As a result, VNIR diffuse body reflectance spectroscopy was able to categorise ripened kiwifruit (*Actinidia deliciosa* "Hayward") by preharvest treatment [17, 11] more effectively than other properties such as mass, hue, dry matter and soluble solids. Also VNIR spectra can be used to discriminate between kiwifruit at different ripeness stages. This was achieved without recourse to other measurements, such as tactile firmness, which would exhibit more characteristic of ripening.

5.1 Future Directions

Diffuse reflectance and transmittance spectra of agricultural products contain information about the chemical composition of the product because each of the components has specific absorption properties. A spectrum is a sampling of a continuous function at a set of fixed wavelengths or energies. It is desirable to use a fine sampling in order not to lose information on the detailed structure of the spectrum. However, the fine sampling will give a large correlation between adjacent points in the spectrum.

Using the intensities of the mass spectra directly as input data vectors for the various methods under test showed to be not manageable because of the large dimensionality of the input data space. Another drawback of using intensities directly can be found in the weak correlation between mass spectral peaks and structural properties for different classes of compounds. Former research on the classification of mass spectra revealed that the reduction and transformation of the input data space by spectral features can greatly enhance the performance of classification. The selection of the optimum set of features for each classification problem is a major consideration. It can be resolved in a several ways:

1. by chemometrics, a well-established standard technique embracing the methods of principle component regression (PCR) and partial least squares (PLS);
2. by signal processing techniques, such as FFT transformations, Wavelet transformation;
3. by genetic algorithms (GA) in wavelength selection in infrared spectroscopy.

In the future work, using a variety of source of historical information, such as a single sampling time series and multiple sampling in time, and information from seasonal cycles of climate rules, a connectionist model, based on time series analysis for predicting and forecasting fruit properties at different stages of development from VNIR spectra, is expected to be developed that employs appropriate feature extraction. There are a number of possible extensions and applications and they are currently under investigation.

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