Data Fusion Approaches as a Novel Strategy in Multivariate Analysis of Spectroscopic and Spectral Imaging Information for Non-destructive Food Microbial and Fungal Assessment

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Abstract

Microbial and fungal contamination of agricultural products as major safety challenges are known in recent years. Non-destructive methods for food quality assessment are warmly welcomed by the food industry. Spectroscopic and optical methods provide a large variety of measurement techniques like optical and near-infrared spectroscopy and imaging which have especially high potential for various food quality assessment. The integration of data and knowledge from several sources is known as data fusion. Data fusion approaches have been introduced as powerful and novel strategies for obtaining more reliable authentication models with respect to the results showed using each method separately. In this paper, we have shortly described the data fusion principles and the most prominent application examples in this rapidly growing strategy of knowledge in microbial and fungal quality assessment of agricultural food products.

Key words: Data fusion, Chemometrics, Microbial assessment, Food quality, Multi-way classification.

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Introduction

The consumer's demand for high quality food products is steadily increasing. The quality, especially of agricultural products, is specified in terms of chemical composition, adequate physical properties, safety with respect to microbiological and toxic contamination [52]. Most of the techniques for microbial evaluation are destructive, time-consuming, require skilled laborers, lab equipment or materials which make it expensive [36, 37, 42]. Thus, it is important to develop non-destructive, accurate, quick and most important valid detection method for microbial contamination. In recent years, there have been growing research works in developing non-destructive methods especially optical-based methods for evaluation external and/or internal quality features of different food products [52]. Spectroscopy and spectral imaging technologies have been evaluated for non-destructive quality evaluation of food products. These optical multispectral and hyperspectral measurements and imaging have recently become more and more popular in food measurements because they lend themselves easily to online monitoring of all samples even without touching the samples [21]. The price of the measurement instruments has also decreased so they provide a viable option for the traditional methods. However, analysis of spectral measurements is often not easy and requires expertise [15, 22]. The mathematical and statistical models created might not be general and need to be adjusted to new conditions and products. Nowadays, a typical optical system employs ultraviolet (fluorescence) and visible wavelengths (Vis), near-infrared (NIR) or infrared (IR) areas or a combination of them. Near-infrared spectrum is especially remarkable since it is related to overtones and combinations of such chemical bonds as C–H, O–H, and N–H which have impact on numerous properties of different agricultural food. These methods play important responsibilities in post-harvest management [46, 60]. In addition, these up-to-date techniques are also increasingly being explored and recommended for microbial detection and evaluation of food quality in both physical and chemical features [29, 30]. The challenge today is how to associate not just single variables as it was done in the past, but blocks of them (like measured data from different sources: Multi spectral (MS), NIR, and Hyper spectral (HS), spectra or spectra and image together). The multivariate statistical analysis of fused data from the optical techniques and imaging systems can be a powerful tool for obtaining more reliable results rather than every single one of them [28].

While spectroscopy produces huge amounts of raw data, there is a strong need to automatically process this data to compress it and to find the features that are relevant or correlate to those that are looked for. Data fusion methodologies have been confirmed to be a powerful tools for obtaining more reliable validation models with respect to the results obtained by each technique separately [28, 2 and 13]. In fact, the fusion of the different data acquired can improve the quantity and quality of facts about the individual features among samples. Furthermore, the integration of the different types of data into a single array also allows evaluating the correlation among the different techniques or sensors.

Data fusion calculates at three different levels (low-, mid- and high-level), depending on the objective, number and type of data sets to combine [32]. Graphical representation of the data fusion process for microbial and fungal assessment of agricultural food products is shown in **Fig. 1**. In the low-level, raw measured data from more than one sensor are directly fused (after pre-processing). This level of data fusion has been widely used for the quality assessment of every type of agricultural food products [23, 51]. The main restrictions are a high data volume and the possible majority of one data source over the others. So, it may be possible to misrecognize regions when spectral data are fused. This is partly overwhelmed by the mid-level. In the mid-level, extraction of some features from each data source is achieved. These features are linked to the single array of features. Besides, this level of fusion allows a great interpretation of the results. Mid-level data fusion has been also applied in authentication and quality control of food and beverages [4, 5, 25]. In the high-level fusion, distinct regression or classification models are achieved from each data source. Then, the results from each individual model are shared to find the final uniqueness decision. In this level, combination of both classification and regression models from each data source achieves better result than individual models. High-level data fusion in food analysis has mostly focused on classification approaches. Bayesian inference based on probability estimation is the most used decision fusion technique [56]. These methods has been recently applied to the analysis of several food products in order to differentiate e.g. an organically or conventional production [26, 27] as well as it has been applied to predict sensory attributes [16]. The main aim of this investigate is: To review the principles and applications of the data fusion approaches that have been applied in the last years in the microbial and fungal assessment of agricultural food products.

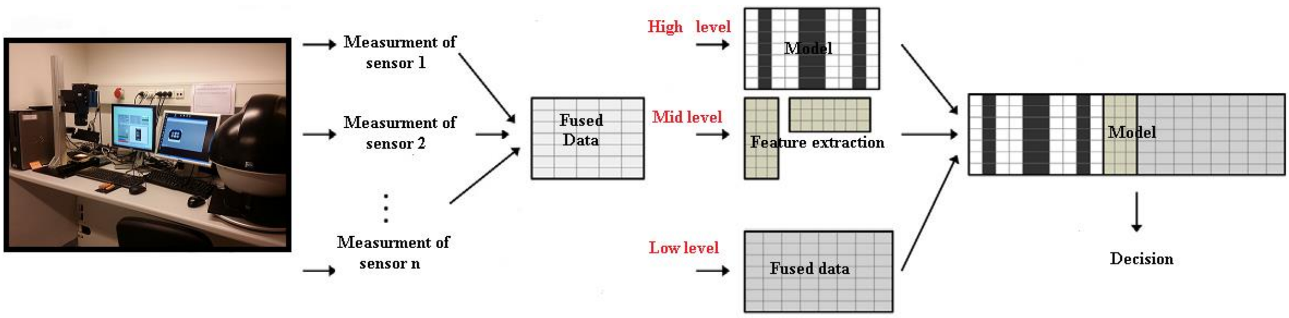

Fig 1. Graphical representation of the data fusion process in microbial and fungal assessment.

Pre-processing in data fusion

In first step of multivariate analysis, different pre-processing techniques on spectra were considered to remove all unnecessary data in the spectra and develop the following classification model or multivariate regression analysis. Data which measured from each sensor depending on their specific characteristics is treated. To this end, standard normal variate (SNV) with multiplicative scatter correction (MSC) were used to remove multiplicative and additive scatter effects, respectively. Also, 1st and 2nd derivatives of the spectrum (D1, D2) based on Savitzky–Golay smoothing filtering with 5 points and two polynomial order were accomplished to enhance the spectral resolution [2]. For intense, standard normal variate (SNV) was used for mid-infrared (MIR) data, multiplicative scatter correction (MSC)was used for near (NIR) and mid-infrared (MIR) spectra [3] and derivatives were used to eliminate baseline shifts in infrared spectra [5], baseline corrections and derivatives were used with UV-vis spectra [10, 11] scaling/normalization with mass spectra (MS) [3,5], and misalignment peak correction with nuclear magnetic resonance (NMR) spectra [14]. Also, low-level data fusion may require further preprocessing methods due to compensate for the different techniques and their measuring scales [16-19]. To this matter, each data from different resources is weighted separately (is called block-scaling) usually with auto scaling, root square scaling and log scaling. Finally, after data are fused, they are usually mean-centered [53].

Multivariate analysis in data fusion

The classification methods most generally used for fusion approaches for microbial assessment and food quality include: linear discriminant analysis (LDA), k nearest neighbors (kNN), Partial least squares discriminant analysis (PLS-DA), support vector machine (SVM), quadratic discriminant analysis (QDA) and Discriminant Function Analysis (DFA), discriminating artificial neural networks (ANNs), Canonical variate analysis (CVA), classification and regression trees (CART), k nearest neighbors (kNN), Orthogonal projection analysis (OPA) as class discriminating techniques [4, 6, 8, 9, 12, 20, 35, 48, 43] and unequal class models (UNEQ), soft independent modeling of class analogy (SIMCA) as classification modeling techniques [55]. Also, the prediction model are principal component regression (PCR), multiple linear regression (MLR) and SVM regression [57]. But, Partial least squares regression (PLSR) is known as the most popular latent variable regression method among them [13].

Variable selection in data fusion

In terms of practical applications for an automatic on-line classified system, working with only one simple sensor in the optimal wavelength ranges, it is important to remove irrelevant and unreliable variables which also improves statistical properties. Both accuracy and speed as a result of using selected optimal wavelengths can be assured. Since the various methods may produce blocks of data with a very different number of variables, predominance of one large matrix over the others may decrease the performance of low-level data fusion [44, 45]. For this reason, data reduction is recommended. The combined data matrix can still have a huge dimension and hold redundant info from the different methods. The most common variable selection method is stepwise selection, where variables are chosen to enter or leave the model following a selected criterion. Stepwise strategies include forward stepwise, backward stepwise or forward entry and backward removal. In the forward methods, variables successively enter the model, whereas in the backward methods the variables are successively removed from the model [1]. Variable Importance in Projection (VIP) scores and selectivity ratios for PLS models separate variables depending on the importance of their information on parameters of the model [12, 14 and 60]. When data are highly correlated, regions of variables are selected instead of single variables. Interval PLS (iPLS), Clustering around latent variables (CLV) uses hierarchical cluster analysis, (ANOVA) variable selection, kernel functions using predefined response 'bell-shaped-windowing' curves and Genetic algorithms (GAs) are assembly of exploration methods [45].

Feature extraction in data fusion

In mid-level data fusion, the features extracted from the different sources are fused to build a single data array which is then analyzed by chemometrics methods. The feature extraction process is useful to reduce dimensionality and keep the relevant information when data volume is still large after variable selection. Principal components or latent variables from PLS-DA commonly used for feature extraction. Nevertheless, other methods like PARAFAC [27], multivariate curve resolution (MCR) [33], kernel based methods [50], independent component analysis (ICA) [7], multiblock methods, such as hierarchical PCA/ PLS, multiblock PCA/PLS or serial-PLS [24] and wavelet transform, also used [59]. For computer vision (CV) systems, specific feature extraction is performed from images based on RGB color mode [43].

Application of data fusion

Multisource information fusion can capture more widespread and unified information about the variety of the object. Single assessment method can only provide one of the features for sample quality assessment. Therefore, multisource information fusion can offer various aids in quality assessment of agricultural products [58]. It is of great interest to explore the feasibility of the sensor fusion approaches for detecting microbial and fungal contamination in different agricultural products [11].

The approach of combined image processing with spectra analysis was successfully developed to identify defective strawberries (bruised and fungal infected) using hyper spectral reflectance imaging system. Hyper spectral image data was exploited by minimum noise fraction (MNF) transformation for strawberry defects distinguished by combining thresholding and morphology procedures, and defective regions were located and separated for spectra extracting. Both linear and non-linear algorithms were developed to identify defective types in strawberries. The results indicated that based on full wavelengths, SVM model performed the highest overall identification accuracy, with the accuracy of 96.91% for calibration and 92.59% for prediction of the fruit [41]. The volatile compounds emitted by the fruits were analyzed by an electronic nose (E-nose) and gas chromatography–mass spectrometry (GC–MS). Principal component analysis (PCA) showed a clear discrimination in decay on day 0, day 2 and day 4 and the infection type on day 2 after fungal inoculation based on 5 selected sensors of E-nose. The discrimination accuracy of the fungal infection type of strawberry fruits for the four groups reached 96.6% by using multilayer perceptron neural network model [49].

The non-destructive method developed based on hyper spectral imaging (HSI) and electronic nose (E-nose) to rapidly detect microbial content and quality attributes of strawberries during decay, was evaluated. Principal component analysis (PCA) was applied to reduce the dimensionality of the data and to extract featured information from the HSI and E-nose data. Quantitative prediction models were developed to forecast the microbial contents and the quality attributes of strawberries. The model constructed based on the raw information fusion of HSI and E-nose data did not improve the prediction accuracy. By contrast, the model constructed based on featured information fusion with essential PCs had better prediction performance than that constructed based on single dataset (HSI or E-nose). The best prediction model was able to predict colony-forming units with a 0.925 RP 2 and RMSEP of 0.38 log10 (CFU g−1) [40].

Total volatile basic nitrogen (TVB-N) content is an important reference index for evaluating pork health. In this investigation attempted to measure TVB-N content in pork meat using integrating near infrared spectroscopy (NIRS), computer vision (CV), and electronic nose (E-nose) techniques. Back-propagation artificial neural network (BP-ANN) was used to construct the model for TVB-N content prediction, and the top principal components (PCs) were extracted as the input of model. The result of the model was achieved as follows: the root mean square error of prediction (RMSEP) = 2.73 mg/100g and the determination coefficient (R_p (2)) = 0.9527 in the prediction set. Compared with single technique, integrating three techniques, in this paper, has its own advantage [31].

A novel sensing system by combining two types of micro sensors, an artificial flavor sensing system has been developed for microbial spoilage in liquids. Initial tests conducted with different liquid samples, i.e. water, orange juice and milk (of different fat content), resulted in 100% discrimination using principal components analysis; although it was found that there was little contribution from the electronic nose. [39].

In the other research, feature level and decision level multisensory data fusion models, combined with covariance matrix adaptation evolutionary strategy (CMAES), were developed to fuse the Enose and zNsose data to improve detection and classification performance for damaged apples compared with using the individual instruments alone. Principal component analysis (PCA) was used for feature extraction and probabilistic neural networks (PNN) were developed as the classifier. The research indicated that the feature selection using the CMAES is an indispensable process in multisensory data fusion, especially if multiple sources of sensors contain much irrelevant or redundant information. At the decision level, Bayesian network fusion achieved better performance than two individual sensors, with 11% error rate versus 13% error rate for the Enose and 20% error rate for the zNose. It is proved that both the decision level fusion using a Bayesian network feature level fusion with the CMAES optimization algorithms as a classifier upgraded performance of model classification [38].

It has to be noted that, in the case of using all low, mid and high levels of data fusion (using different strategies : variable selection or feature reduction), it is necessary to end up with comparing data obtained from each single data resource analysis.

Conclusion

This paper reviews shortly the basic of data fusion principles and the most noticeable application examples in microbial and fungal assessment of agricultural food products. Data fusion is recognized as the process of getting data from multiple sources with the aim of build more sophisticated models and get more details about a target. Various types of data fusion (identify low, intermediate and high-level data fusion) work in different ways. Unfortunately there are a few many works in the data fusion strategy of microbial and fungal assessment for agricultural foods that we were able to consider only a small fraction of the total literature existing about other food qualification dimensions, which means that too many important contributions had to be done in this area. Nevertheless, the authors hope that this paper could help those who are trying to find explanations or model methodologies to their food microbial and fungal assessment problems from optics, imaging, and spectroscopy methodologies.

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