15-1214

Chemometrics

Applications Overview

Chemometrics in Food and Beverage

Abstract

Scientists in the food and beverage industry are faced with many different quality control tasks, such as making sure that flavors meet certain standards, identifying changes in process parameters that may lead to a change in quality, detecting adulteration in any ingredient and identifying the geographical origin of raw materials. Food scientists who work for regulatory agencies, such as the Food and Drug Administration, are interested in detecting economic fraud due to product substitution and adulteration, as well as health risks from possible contamination.

Many of these quality control issues have traditionally been assessed by experts, who are able to determine a product's quality by observing its color, texture, taste, aroma, etc. However, it takes years of experience for one to acquire these skills. It would therefore be advantageous if there were a way for food scientists to measure the quality of a product by instrumented means.

Unfortunately, quality is a difficult parameter to quantify. It is difficult to find direct sensors for quality parameters such as freshness or expected shelf life; therefore we are forced to measure an indirect set of parameters which, individually, may be only weakly correlated to the properties of interest. In analyzing this multivariate data, patterns emerge which are related to product quality and can be recognized by either a human interpreter or a computer.

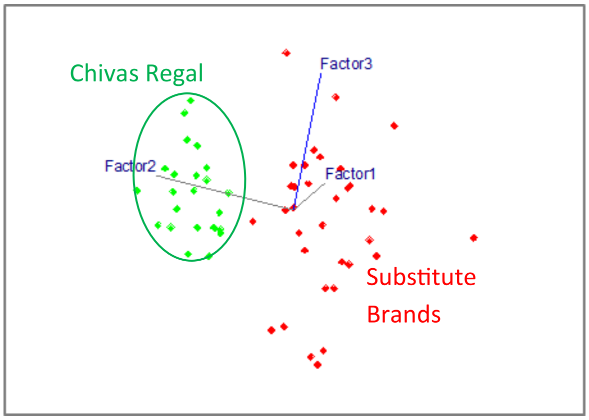

Figure 1. Whisky samples can be classified based on the relative composition of trace constituents (21)

For example, a chromatogram or spectral profile can be thought of as a fingerprint, where a pattern emerges from the relative intensities of the chromatographic sequence or spectrum. If these fingerprints are repeatable for every batch packaged for sale, it is possible for an automated quality control system to interpret those patterns in the data.

Chemometrics is a statistical approach to the interpretation of patterns in multivariate data. When used to analyze instrument data, chemometrics often results in a faster and more precise assessment of composition of a food product or even physical or sensory properties. For example, composition (fat, fiber, moisture, carbohydrate) of dairy products or grain can be quickly measured using near infrared spectroscopy and chemometrics. Food properties (*e.g.*, taste, smell, astringency) can also be monitored on a continuous basis. In all cases, the data patterns are used to develop a model with the goal of predicting quality parameters for future data.

The two general applications of chemometrics technology are:

- to predict a property of interest (typically adherence to a performance standard); and
- to classify the sample into one of several categories (e.g., good versus bad, Type A versus Type B versus Type C ...)

Food and Beverage Applications

This overview describes several applications in which chemometrics software has simplified methods development and automated the routine use of robust pattern matching in the food and beverage industry. The examples cited can be duplicated using Pirouette® multivariate modeling software and automated in a routine quality assurance setting using InStep™.

Process Monitoring and Control

- Grading of raw materials (1)
- Routine on-line quality checks (2, 3)
- Minimizing sample preparation (4)
- Determining process by which product was made (5)

Much of the research and the quality control effort are aimed at assessing a product's consistency or identifying changes in process parameters that may lead to a degradation of quality standards. In most cases, no single measurement is sufficient to categorize samples for QC purposes. By examining a series of parameters simultaneously, an instrumental technique can be utilized that is considerably more precise than the manual spot quality checks that are the tradition. The speed and efficiency of the instrument allows chemometrics technology to be used for batch-to-batch product control (6).

Chemometric profiling is useful for detecting changes in a process or in the ingredients; it can also be used to monitor plant-to-plant product variations. For example, near-infrared

(NIR) spectroscopy can be used to determine the moisture content in packaged and prepared goods such as baking dough. NIR can also be used to monitor the carbohydrate content of grains and other natural products, which vary in composition, as they are processed. The chemometric technique has even been applied to the classification of products based on their nutritional makeup (7).

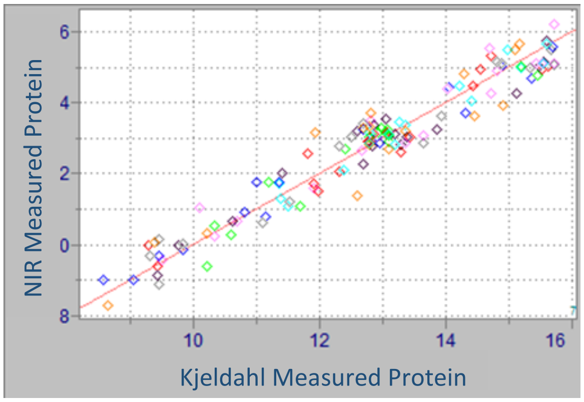

Figure 2. Compositional parameters such as the protein, moisture and fiber content of raw or manufactured food products can be monitored using near infrared spectroscopy and chemometrics

Geographical Origin

- Identifying origin of contamination
- Determining source of ingredients by chemical composition (8)
- Tracing origin of finished products by flavor and aromatic components (9)

Chemometric pattern matching has been used in a wide variety of applications where the origin of a sample is in question. For instance, in developing a chemometric model for quality control of orange juice, two distinct groups of juice samples were shown to originate from different geographical locations (Florida and Brazil). The article demonstrated that chemical composition could be used to trace the origin of the fruit (22).

Similar work in identifying a product's origin has been reported for olive oils (10), brandy (11), wine (12) and mineral water (13). Another study demonstrates that it is possible to relate composition patterns in wine to the wine region and the vintage year (14).

Sensory Evaluation

- Classification by flavor profiles (15, 16)
- Replacing sensory evaluation with instrumented analysis (17)

A major thrust in the food and beverage industry is to bring analytical instrument techniques to play in sensory evaluation. Traditional sensory panels are expensive to maintain and can lead to inconsistent conclusions. This subjective approach to quality control can be (to some extent) replaced or enhanced by collecting chromatographic and spectroscopic information that have a high degree of correlation to sensory parameters.

Taste, smell, astringency, etc., are related to fats, oils, esters, proteins, minerals, aromatics and carbohydrates present in food. Many of these components can be profiled (fingerprinted) by instrumented techniques and then correlated to sensory information by chemometric methods. The resultant statistical model can be used in on-line or routine applications to predict flavor characteristics of unknown samples via the same instrumented technique.

Economic Fraud

- Identification of product adulteration, dilution and contamination (18, 19, 20)
- Detection of substitution (21)

It is an unfortunate fact of life for many food producers that competitors may attempt to undercut their business by selling an adulterated product. Similarly, a less expensive, lower quality product is sometimes substituted and labeled as a more expensive product.

As an example, it has been shown that adulteration can be detected in orange juice using trace element data and chemometric techniques (22). Data were collected for both orange juice and grapefruit juice, a common adulterant in "100% pure" orange juice. A chemometric model, or fingerprint, was created for each type of juice and for a blend of both juices. The model was then applied to data for new juice samples in order to determine product purity.

Another example is the unnecessary addition of water to grain. Is the amount of water added by grain resellers appropriate for dust control or is it actually economic fraud (higher weight, thus higher profit)? Monitoring the product by near infrared spectroscopy and analyzing this data with chemometrics could produce a real-time, inexpensive monitoring device (23).

Chemometrics can be used to identify instances where rockfish might be packaged and sold as red snapper. Chromatographic techniques are employed to collect data for both red snapper and rockfish; the data are then analyzed to create fingerprints for both types of fish. The model, shown in Figure 3, evaluates samples of fish to detect mislabeling. This system can be employed to verify that a particular chromatographic profile matches the red snapper fingerprint.

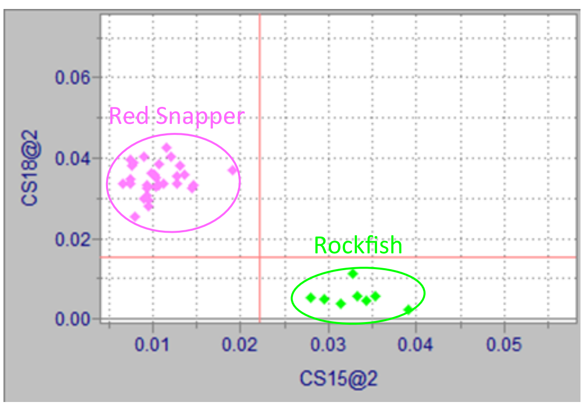

Figure 3. The profiling of seafood samples can detect the substitution of rockfish (class 18) for red snapper (class 15)

Summary

Chemometrics is a statistical technique that can directly correlate quality parameters or physical properties to analytical instrument data collected on food products. Patterns in the data are modeled; these models can then be routinely applied to future data in order to predict the same quality parameters. The result of the chemometrics approach is an efficiency gain in assessing product quality. The process can lead to more efficient laboratory practices or automated quality control systems. The only requirements are an appropriate instrument and software to interpret the patterns in the data.

Chemometrics software is designed to recognize patterns in virtually any type of multi-dimensional analytical data. Chemometrics can be used to speed methods development and make routine the use of statistical models for data analysis. Specifically, the application of chemometrics to the quality control of food or beverage products results in:

- More comprehensive monitoring of product quality and changes in process parameters
- Routine monitoring of raw material quality including assessment of geographical/varietal origin
- Replacement or augmentation of sensory evaluation with analytical instrument systems
- More efficient detection of product adulteration, contamination and substitution

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