Trends in chemometrics and meat products

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Abstract. Chemometrics is a set of mathematical and statistical methods that are used to detect food fraud, predict microbial growth, and optimize design of experiments, while extracting useful information from large and complex datasets. Complex datasets quite often have numerous sources of variations, with one or more dependent variables assessed against the two or more dependent variables, hence the need to employ some type of multivariate statistics. It is critical to decrease the chances of type I error, by comparing (calculating) all the effects of independent variables in a single multivariate test. The most common types of multivariate tests include multivariate analysis of variance (MANOVA), various forms of factor analysis (such as principal component analysis, PCA), and mathematical modeling. Bioactive compounds of plant origin possess desirable health benefits and hence are interesting for functional meat processing. The extraction and processing of bioactive compounds mostly revolve around the central problems of thermal (in)stability and environmental issues that are relevant for industry. Here, multivariate statistics can offer the best mathematical solutions for optimal industrial production or can devise various indexes that are able to follow changes of the entire chemical footprint during the extraction of target compounds. For instance, multivariate statistics is useful to determine optimal extraction parameters for antioxidants, while simultaneously evaluating the effects and interactions of extraction parameters.

1. Chemometrics in food science

Meat is one of the main sources of proteins, and its global production and processing will increase in the future [1]. As any food product on the market, processed meats must have required organoleptic, physio-chemical and food safety characteristics.

Significant developments in (instrumental) laboratory equipment have converted bench sciences like chemistry into great data generators while providing food science professionals with large amounts of data and a new problem, i.e., how to make sense of all that data [2]. As a solution, data analysts have
resorted to statistical concepts and tests cumulatively known as multivariate statistics that employ simultaneous analysis of one or more dependent variable(s) against two or more independent variables [3]. The key point here is “simultaneous comparison”, which if not used, has a tendency to inflate type I errors, meaning the data tend to falsely show effects and significances that do not really exist [4].

Dependent and independent variables can be categorized as qualitative or quantitative [5], whereby the former includes nominal (e.g. four types of meats; three types of meat seasoning); dichotomous (e.g. authentic or adulterated meat product; male or female animal), and; ordinal variables (e.g. data with some ordering, like the levels of a hedonistic scale for sensory evaluation of prosciutto). On the other hand, the latter, quantitative variables include scales, intervals, and ratios [6]. For example, in meat science, scales include length of processing in minutes, temperature of curing ham, added quantities of salt in brine etc. Intervals and ratios correspond to terms commonly used in everyday life.

Chemometrics encompasses the use of multivariate statistics and data mining to obtain valid conclusions from large data sets [7]. Multivariate tests include but are not limited to multivariate analysis of variance, numerous factor analyses (e.g. principal components analysis; PCA), mathematical modeling, and discriminant analysis [8].

Recently, chemometrics has been applied by government agencies and food industries to tackle the problem of food fraud and public concerns about the safety and quality of foods [9], to determine optimal processing parameters for various conditions and raw materials [7, 10], and to solve other problems in food science. This review aims to give a brief overview of the use of chemometrics in meat processing, focusing on mathematical modeling and PCA as the most commonly used multivariate tools in food science.

2. Mathematical modeling of food processing and food safety

Currently there is a demand for fresh and natural products that are safe for consumption [11] but have the least possible amounts of synthetic additives [12]. This has led to the synthetics being replaced with natural alternatives that are usually extracted from plants (fruits, vegetables, agri-food waste, medicinal plants etc.), along with the development and application of processing techniques able to reach and retain desired levels of microbial load. With savvy food engineering, such products can also be labeled as “functional foods” and placed in the largest growing food marketing segment worldwide. Either way, there is an objective need for optimizing extraction procedures for bioactive compounds and predicting the microbial content of food products, and these needs are an important segment of food manufacturing [13]. One efficient way to achieve such goals is to use mathematical modeling.

Mathematical modeling is a common chemometric (multivariate) approach used in food science and technology to decrease experimental costs, predict outcomes, and optimize and describe complex processes [14]. Usually it has two main stages, construction and testing of potential mathematical relations [7] that are preceded with experimental design to achieve an optimal number of experimental runs [15]. The main purpose of modeling is to construct equations that are able to give good estimates of complex phenomena in a simplified manner [16]. Based on the method used, the equations constructed can be categorized as fundamental (mathematical regression) or semi-fundamental (Michaelis-Menten, Arrhenius, or predictive kinetics) models [14].

Fundamental modeling is usually done with some form of regression analysis that builds mathematical relations from raw data, and often from a large number of parameters [14]. The sheer amount of data and parameters makes it difficult to find and build relations, while an additional need is for experienced data analysts with solid statistical backgrounds to achieve such tasks. On the plus side, the fundamental models obtained are tailor-made for particular situations while being accurate and flexible [16].

Semi-fundamental models are simpler but less accurate and versatile, as they assume that one or more parameters are insignificant or constant [16].

Some examples of modeling processing parameters to obtain plant extracts that can act as natural additives in meat products have been recently reviewed [12]. These mixtures of various biologically active compounds need to contain the highest possible amounts of antioxidants [17], but thermal
degradation of the compounds during extraction should be avoided [18]. To optimally achieve that, the extraction technology employed [19] must be optimized by mathematical modeling [20]. Details comparing the advantages and disadvantages of processing technologies were reported elsewhere [21]. The example of microbial growth in meat was recently reviewed [22], and methods for managing microbial spoilage in the meat industry were previously reported [23].

3. PCA and meat adulterations
Aside from food safety and quality, consumers require authentic food products. Food adulteration is a very complex and worldwide problem, causing scandals and economic losses [24, 25] and even having severe repercussions for human health [26]. For instance, meat products are particularly interesting for fraudulent activities, for example, to the extent that corruption was shown in Brazil’s government food safety system, when meat contaminated with Salmonella was served in Brazilian public schools [7]. Government, law enforcement agencies, media, and other professionals should work together to suppress food adulteration; however, all of them rely on specific information to be able to successfully do their jobs and implement the law [9, 27-29]. Here is yet another application of chemometrics, i.e. the very useful analysis of biological and chemical markers able to form a fingerprint for a particular attribute of a food. The fingerprint could, for example, define place of origin, batch, foreign components, etc. [30]. The concept behind detecting food fraud relies on comparing the fingerprint of an authentic food with that of a suspicious counterpart [31]. Factor analysis is a data tool that can be used in detecting food adulteration of meat products and their compliance with legal requirements [32-34].

PCA is one of many factor analysis methods, with the main purpose in food science of finding underlying relations among biological and chemical markers from large datasets [35]. During the process of PCA, it is important to define only those variables that are useful for detecting adulteration in the food, or to reduce the dataset to use only statistically relevant variables for forming the adulteration fingerprint (index). Hence, this procedure is also called reduction of dimensions. Some examples of using PCA to detect adulterated meats include minced lamb with duck meat [36, 37], wild deer with domestic goat meat [38], and beef with horse meat [39].

4. Conclusions
In conclusion, current trends show that chemometrics has various versatile applications in the analysis of large datasets that are provided by powerful, new laboratory techniques. Among the most interesting applications are optimizing the methods of processing bioactive food additives, predicting microbial growth with the aim of improving food safety and detecting/preventing adulteration of foods by analyzing biological and chemical biomarkers.

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