Application of Partial Least Square analysis (PLS) and General Procrustes analysis (GPA) in understanding the relationships between sensory descriptive and headspace flavor profiles.

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Flavor perception is a highly complex system. Flavor can be perceived retronasally only when the odor-active volatiles are released from food to the buccal headspace during mastication. Flavorful foodstuffs can include hundreds of volatile compounds. In addition, these volatiles are not uniformly released from the food, but may interact with macro ingredients such as fat, carbohydrate, and proteins of the food base in many different patterns. Although often a large number of flavor volatiles are involved in stimulating human senses, the number of sensory flavor descriptors generated during food consumption is much smaller, which makes the direct correlation of volatiles with flavor descriptors difficult. However, multivariate techniques can be effectively applied to drawing relationships between volatile profiles and sensory descriptive data. Dijksterhuis (1994) classified the statistical methods into asymmetric and symmetric methods. The former methods (e.g. PLS) are capable of predicting one data set from the other data set while the latter methods (e.g. GPA, Canonical Correlation analysis) simply describe the relationship between the data sets. PLS is a hybrid method of multiple regression and Principal Component Analysis (PCA) (MacFie and Hedderley, 1993). GPA extracts a common structure from multiple data sets composed of non-identical variables between the data sets.

In this paper, a very effective statistical strategy using these two multivariate analyses is illustrated to link the sensory perception to the flavor profile obtained by dynamic headspace analysis. Ice cream with varying fat levels (0%, 3%, 6%, and 12%) was used as the vehicle for the flavor compounds in the experiment. The ice cream base was spiked with known amounts of 3 different volatiles (hexanal, vanillin, and delta-decalactone). Descriptive Analysis (DA) of the samples was conducted using 11 panelists, who evaluated the samples using the texture and flavor descriptors generated during the training sessions. Instrumental analysis was conducted on the same samples by extracting volatiles using a dynamic headspace method. The volatiles extracted from the samples were analyzed by Gas Chromatography-Mass Spectrometry (GC-MS). The areas of volatile peaks from the GC chromatogram were used for the statistical analyses.

Sixteen flavor and texture attributes were generated from DA. Fifty-eight volatile compounds were initially identified from GC chromatograms. The number of volatiles was reduced to 22 based on significant differences between various fat levels and PC loadings by GLM and PCA, respectively. These selected volatiles were then further studied to investigate their impact on the sensory profile of ice cream using GPA and PLS. Due to the concern of the existing large-scale differences between sensory and chemical data sets, another chemical data set was generated by log-transforming the chemical data. Initially, GPA and PLS was performed using the DA and untransformed chemical data sets (CHEM). The same statistical analyses were then conducted using DA and log-transformed chemical data sets (LCHEM). The results from the two statistical analysis methods were compared and the effect of log-transformation on the overall chemical-sensory relationship was evaluated within each statistical method.

A combination of flavor compounds successfully predicted the sensory attributes in PLS using CHEM-DA data sets. Models generated by PLS also gave a predictive level for each sensory attribute based on cross-validation methods. Alcohols, hydrocarbons, and aldehydes contributed to sensory characteristics (i.e. icy, stale, crumble, and fast melt rate) of low and non-fat ice creams. Ketones, such as 2-hexanone, 2-heptanone, and 2-nonanone which have fatty, soapy, or hot milk flavor qualities, were driving the sensory characteristics of high-fat ice creams. In the PLS model, these ketones were more related to cream flavor, cooked flavor, vanilla, eggy flavor, denseness, thickness, and mouth coating. Because intuitively, flavor volatiles should have high correlation only with flavor attributes, observing high correlation between flavor compounds and texture attributes is surprising. However, it is important to realize that the underlying sample structure was controlled by the "fat level" in this experiment and that fat controls the release of flavor, as well as the physical characteristics of ice cream. Unlike the analysis of CHEM-DA data sets, PLS for LCHEM-DA data sets were not able to sufficiently predict the effect of flavor compounds on the sensory attributes of ice cream flavor.

GPA gave similar statistical results to that obtained from PLS. In the GPA for CHEM-DA, hexanal, which was intentionally spiked in high amounts into some of the samples in the experiment, stood out in the GPA plot indicating that the GPA structure was significantly driven by hexanal and stale flavor. For LCHEM-DA data, GPA separated the samples and the variables better than PLS did. GPA weighted all the chemical compounds similarly to each other after log-transformation, and thus enabled us to see the relationships between the sensory and overall volatile profile patterns.

PLS and GPA were both successfully used to draw linkages between the chemical and sensory data with similar results. PLS had the advantage of predictive performance. Log-transformation of the chemical data was disadvantageous when using PLS. However, for GPA, log-transformation can be useful in delineating the chemical-sensory relationships when initially the volatile compounds are not weighted similarly to each other.

References

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