

Multivariate modelling of sensory profiles (Flavoured waters)

Challenge

Identifying the factors that have an impact on the design of a product (with specific sensory profile) for a beverage manufacturer wanting to develop and introduce a flavoured water that will succeed in the market.



Solution

Perform full factorial design to specify test samples that span the variation in design. Qualify and calculate the average sensory profiles and perform PCA to identify the factors that impact.

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A beverage manufacturer wants to introduce a new type of flavoured water to the market. In the first stage of product development, he wants to compare a set of test samples using a trained sensory panel.

Water samples

Design of Experiments (DoE) is the best way to specify test samples that span the variations we are interested in. Eighteen water samples were prepared according to a full factorial design set up by The Unscrambler® software. Three factors were varied in the design: Flavour type (2 levels), flavour dosage (3 levels) and sugar content (3 levels). The design samples are illustrated in Figure 1.



Principal Component Analysis (PCA) is a powerful method for summarizing variation in many variables.

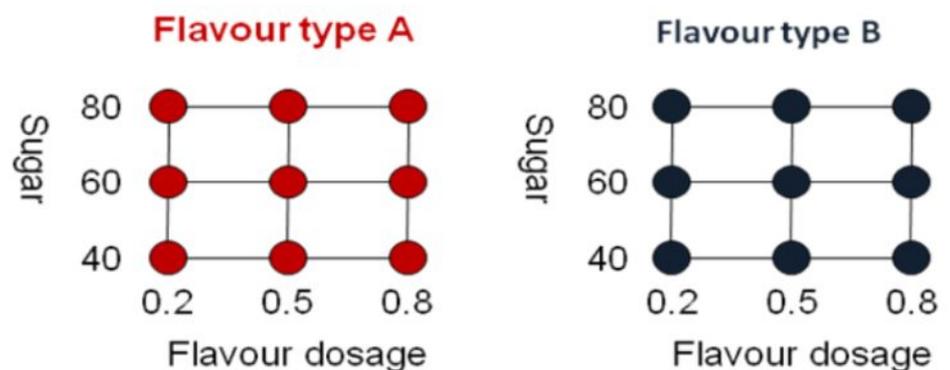


Figure 1: Full factorial combinations of flavour type (2 levels), sugar content (3 levels) and flavour dose (3 levels).

Sensory evaluations

An expert sensory panel consisting of 11 panelists evaluated the water samples. Twenty-three attributes were scored on a scale from 0 to 10, and each panelist tasted all samples twice. The sensory scores were evaluated using the QualiSense software, and four attributes were removed due to low sensitivity. One severe cross-over error was also corrected, before the average sensory profiles were calculated.

Multivariate data analysis

Principal Component Analysis (PCA) is a powerful method for summarizing

variation in many variables, for example sensory profiles. PCA projects the main variation onto a few Principal Components (PCs), meaning that the samples and variables can be compared and interpreted through simple, two-dimensional maps. The sensory profiles of flavoured waters were analysed by PCA using The Unscrambler® software.

The map of samples is called Scores and the map of variables is called Loadings. A variant of the traditional Loadings plot is the Correlation Loadings plot, which shows the correlation between the PCs

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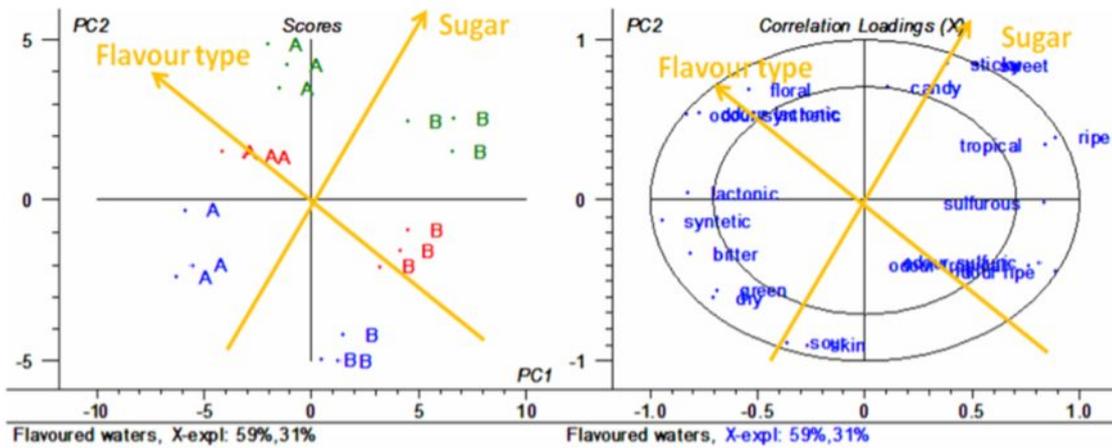


Figure 2: Scores (left) and Correlation Loadings (right) show the relationships between samples and variables respectively. These plots show PC1 versus PC2, summarizing 70% of the variation between waters. The colours in the score plot represent sugar levels (blue=low, red=medium, green=high). There is a clear pattern due to flavour type (A or B) and sugar levels, shown by the yellow arrows.

and the original variables. Scores and Correlation Loadings for PC1 versus PC2 are shown in Figure 2.

There are two clearly separated groups of samples in the score plot, corresponding to flavour types A or B. This means that the two flavour types give waters with significantly different sensory profiles. The direction of difference between A and B is indicated by a yellow arrow in the plot. The same direction in the loading plot reveals which sensory attributes are different for the two flavour types. We see that type A is

characterized by attributes floral, odour synthetic and odour laconic, while type B is described by attributes ripe, odour sulphuric and odour tropical.

The colours in the score plot represent low, medium and high sugar levels. There is a clear systematic trend corresponding to sugar levels, which means that it has a significant effect on the sensory profiles. The direction of increased sugar level is indicated by an arrow in the score plot, and the corresponding direction in the loading plot shows that low sugar level

gives waters which taste like sour, skin, dry and green. High sugar levels give waters which are sweet and sticky.

There is no pattern due to flavour dosage in the first two PCs. If we look at the score plot of PC1 vs. PC3 (Figure 3), we can notice that most of the low dosage waters (blue colour) are in the lower part of the plot, while medium and

high are in the upper part. This indicates that there is a small difference between low and medium dosage, but no difference between medium and high. Note that PC3 only explains 2% of the variation in sensory profiles, which means that the dosage effect is negligible compared to the effects of flavour type and sugar.

Conclusion

The multivariate analysis identified the factors that have an impact on the sensory profiles, and the attributes that are affected. This knowledge can be used to “design” waters with a specific sensory profile.

Flavour type has a strong effect on the sensory properties of the waters. Flavour type A has a floral taste and synthetic and lactonic odour, while type B tastes ripe and smells tropical and sulphurous.

Sugar content also has an effect on the sensory profiles. Not surprisingly, the waters go from sour, skin, green and dry to sweet and sticky when sugar is added.

Flavour dosage does not seem to affect the sensory profiles much. There might be a small difference between low and medium dosage, but even if the difference is systematic it is so small that it has little impact in practice.

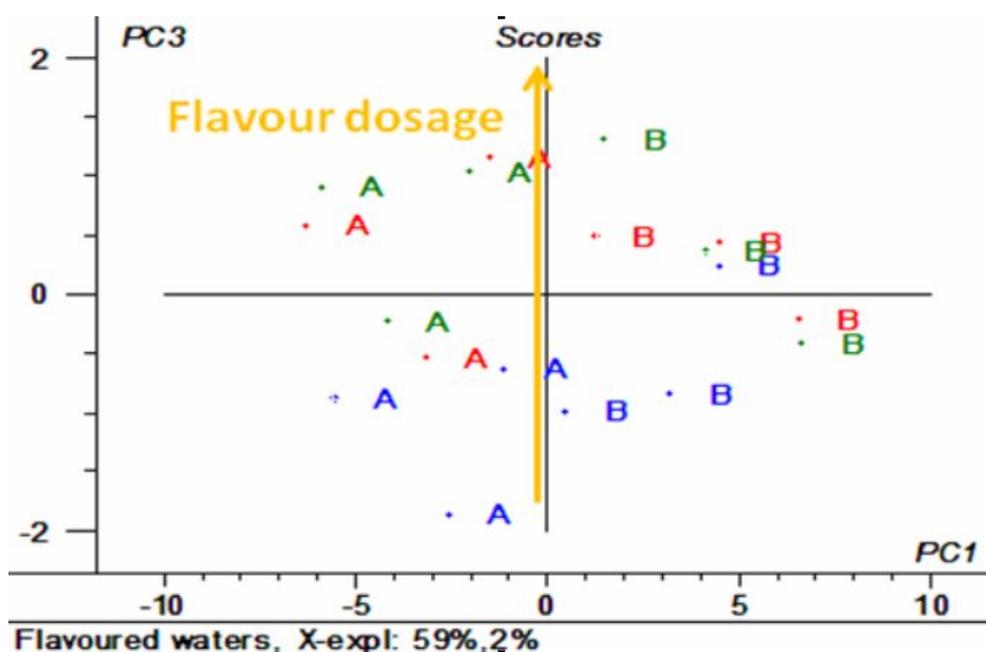


Figure 3: Score plot for PC1 vs. PC3. The colours represent flavour dosage (blue=low, red=medium, green=high). Most of the low-dosage waters have low values in PC3, but PC3 only explains 2% of the variation in sensory profiles.

Application note overview

Software	The Unscrambler 9.7®
Methods	DoE and PCA
Data type	Sensory profiling data
Industry	Food and Beverage
Added Value	The sensory panel scores were validated and can thereby confidently be used for decision-making and further data analysis.