1. Introduction

Directly relating aroma composition and concentration data to the perceived aroma quality and intensity present several challenges:

- The aroma concentration is not linearly related to the perceived aroma intensity (sigmoid relation).
- The absolute abundance of each volatile compound can impact differently the perceived aroma quality and intensity.
- Human nose seems more able to identify volatile molecule patterns due to relative abundance than aromas through direct relations to absolute abundances (Menini, 2009).

2. Transformation procedure

A transformation of the raw analytical data is required to obtain an estimate of the aroma pseudo-composition which is meaningful to relate with the sensory profiles. The transformation procedure is described in 4 steps.

**Step 1: Log-transformation**

Log-transformation of the raw data +1 to avoid that values inferior to 1 get an overestimated weight.

- Raw data
  - Product 1
  - Product 2
  - Product n
- Normalization
  - Mean
  - SD

**Step 2: Normalization**

Standardization of the log-transformed data in order to put all compounds on a similar scale of values.

- Raw data
  - Product 1
  - Product 2
  - Product n
- Normalized data
  - Mean
  - SD

**Step 3: Pseudo-concentration**

Aroma pseudo-concentration estimate to compare the relative abundance of volatile compounds between products.

- Normalized data
  - Product 1
  - Product 2
  - Product n
- Pseudo-concentration
  - for i = 1, ..., n & j = 1, ..., p

**Step 4: Pseudo-composition**

Aroma pseudo-composition estimate to express aroma compounds in terms of relative abundance with respect to the overall load of aroma molecules.

- Raw data
  - Product 1
  - Product 2
  - Product n
- Pseudo-composition
  - for i = 1, ..., n & j = 1, ..., p

3. Procedure to relate transformed data and sensory

The sensory profiles are mapped on a biplot by using the Principal Component Analysis (PCA) with the sensory data. The aroma pseudo-compounds are then overlapped on the map as supplementary variables.

- Products (in blue) are mapped on the biplot based on their sensory profile.
- Sensory attributes (in grey) are represented by arrows on the map.
- Pseudo-compounds (in green) are overlapped on the map as supplementary variables.

This approach has the advantage to give more importance to the sensory space enabling to identify which aroma pseudo-compounds correlate the best with key sensory dimensions.

References


