Proposal of statistical procedure to relate aroma chemistry data to aroma sensory data

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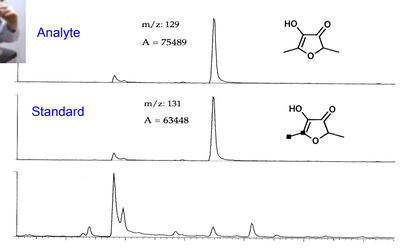
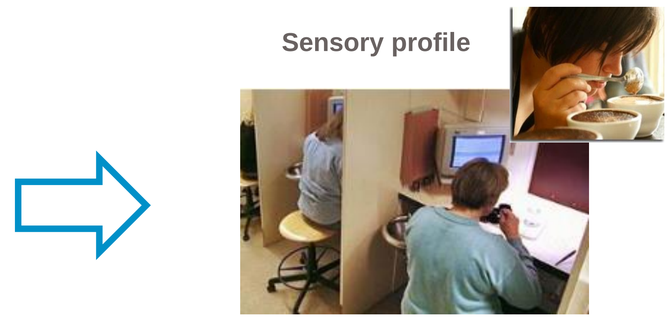
1. Introduction

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)

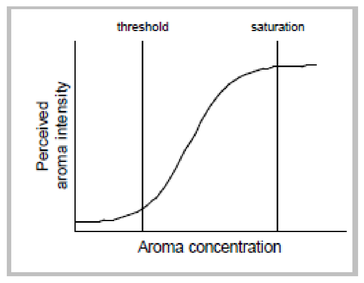
Volatile compounds



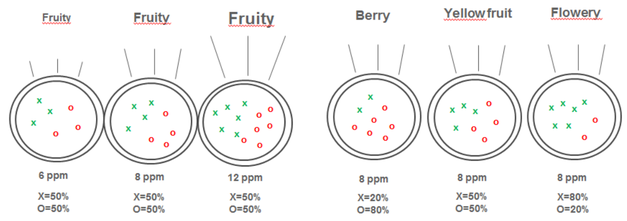


Sensory profile

Sigmoid relation



Aroma concentration and composition are not directly related to perceived intensity and quality



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 0: Data structure

Consider analytical data of the form x_{ij} with:

- $i = 1, \dots, n$ rows (products)
- $j = 1, \dots, p$ columns (compounds)

Raw data	Compound 1	.	.	.	Compound p
Product 1	x_{ij} for $i = 1, \dots, n$ & $j = 1, \dots, p$				
.					
.					
.					
Product n					

Step 1: Log-transformation

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

Log data	Compound 1	.	.	.	Compound p
Product 1	$y_{ij} = ln(x_{ij} + 1)$ for $i = 1, \dots, n$ & $j = 1, \dots, p$				
.					
.					
.					
Product n					

Mean	$\mu(y_{.1})$	.	.	.	$\mu(y_{.p})$
SD	$\sigma(y_{.1})$	.	.	.	$\sigma(y_{.p})$

Step 2: Normalization

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

Normalized data	Compound 1	.	.	.	Compound p
Product 1	$z_{ij} = \frac{y_{ij} - \mu(y_{.j})}{\sigma(y_{.j})}$ for $i = 1, \dots, n$ & $j = 1, \dots, p$				
.					
.					
.					
Product n					

Step 3: Pseudo-concentration

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

Normalized data	Compound 1	.	.	.	Compound p
Product 1	z_{ij} for $i = 1, \dots, n$ & $j = 1, \dots, p$				
.					
.					
.					
Product n					

Pseudo-concentration
$v_1 = \text{mean}(z_{1j})$
.
.
.
$v_n = \text{mean}(z_{nj})$

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

Pseudo-composition	Compound 1	.	.	.	Compound p
Product 1	$w_{ij} = z_{ij} - v_{i.}$ for $i = 1, \dots, n$ & $j = 1, \dots, p$				
.					
.					
.					
Product n					

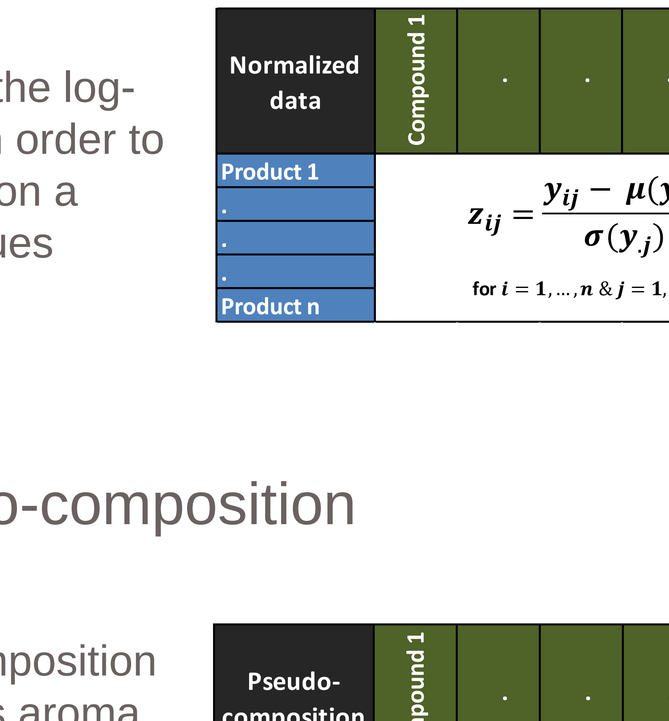
3. Procedure to relate transformed data and sensory

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.

Biplot



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