Underlying dimensions in the descriptive space of perfumery odors: Part II

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ABSTRACT

Some comprehensive compilations of odor character descriptions are available in the literature, and they contain valuable information to better understand the underlying dimensions of human odor psychophysics. In the present study, principal component analysis was applied to two olfactory databases of perfumery materials publicly available, which are comprised by those odor descriptors most frequently used in perfumery. The projection of descriptors over the two principal axes (two-component solution) led to related plots, which are also similar to the one obtained in a previous study (Zarzo, 2008). Although the descriptive space of odors is highly multidimensional, our results suggest that it is possible to reach a consensus about how to project perfumery scents on a two-dimensional map, and how to interpret the dimensions of that sensory map. One of them discriminates light vs. heavy odors; the orthogonal axis was correlated with hedonic tones, but it is better interpreted as an underlying latent structure that distinguishes feminine vs. masculine cosmetic scents.

1. Introduction

Two-dimensional (2-D) representations of flavors are valuable tools for sensory analysis. The beer flavor wheel displays different classes around a central point resembling the radii of a wheel. Classes next to each other are supposed to be similar, while those located in opposite positions represent dissimilar flavors (Meilgaard, Dalgliesh, & Clapperton, 1979). Similar representations have been developed in other areas, like the wine aroma wheel (Noble et al., 1987), the coffee taster's flavor wheel (Lingle, 1992) and the sensory wheel for virgin olive oil (Mojet & De Jong, 1994).

Perfumes are complex mixtures of scents, and their sensory description becomes difficult for naive consumers. With thousands of perfumes available in the market, shopping for a new fragrance can become confusing. In order to allow a better communication between perfume retailers and consumers, it would be helpful to use a standard 2-D sensory map of odor descriptors, which would serve as a basis to understand the classification of fragrances. Unfortunately, such standard map does not exist yet probably because there is not an agreement about the most appropriate scientific methodology to reach a consensus. Perfumery companies have developed different schemes for classifying commercial fragrances, such as the Discodor (Harder, 1979), Analogies of Givaudan (Figs. 3 and 4 of Thiboud, 1991), the Drom Fragrance Circle, the natural perfume wheel of Aftelier (2006), the Rosace of Firmenich, the Hexagon of fragrance families (Haldiman & Schuenemann, 1990), and some others mentioned by Jellinek (1992). Additional sensory maps of scents have been developed by individual perfumers like Jellinek (1997) and Edwards (2010). Despite the amount of available olfactory representations in this field, their comparison is difficult because the relative position of descriptors often differs considerably, and only few odor maps can be matched with a reasonable agreement. The classification of perfumes is an area of scientific interest (Teixeira, Barrault, Rodríguez, Carvalho, & Rodrigues, 2014), but few efforts have been carried out to compare such classifications aimed at providing certain consensus scheme.

The most scientific way to develop a sensory map of scents is to obtain a large compilation of odor descriptions and to analyze them with multivariate statistical methods. Such approach has been carried out by different researchers (Abe, Kanaya, Komukai, Takahashi, & Sasaki, 1990; Chastrette, de Saint Laumer, & Sauvegrain, 1991; Jaubert, Tapiero, & Doré, 1995; Madany-Mamlouk, Chee-Ruiter, Hofmann, & Bower, 2003; Zarzo & Stanton, 2006). However, the sensory maps obtained in these works are difficult to compare. Given such disparity and the fact that odor percepts depend on

prior learning and experience (Li, Luxenberg, Parrish, & Gottfried, 2006; Wilson & Stevenson, 2003), many olfactory researchers even doubt if it is possible to reach a standard map of scents. Actually, as the olfactory descriptive space is structured in at least 10 dimensions (Castro, Ramanathan, & Chennubhotla, 2013), it is uncertain how to project such space over a two-factorial plane. Nonetheless, fragrances are basically cosmetic pleasant scents and, hence, many food flavors are rarely present (e.g. cheese, butter, fish, meat, garlic, etc.) as well as very unpleasant smells like putrid, sulfurous or burnt odors. Although the subspace of fragrances is very broad, reported evidence suggests that perfumery descriptors can be consistently mapped over two meaningful dimensions (Zarzo & Stanton, 2009), but this issue still requires further empirical evidence.

The main target of the present work is to further investigate how to project the multidimensional space of perfumery descriptors over two dimensions and to check if the resulting solution is consistent with other sensory maps of scents previously reported. For this purpose, two comprehensive olfactory databases of perfumery materials are analyzed. Based on the results, three sensory wheels of fragrances are discussed.

2. Materials and methods

2.1. Olfactory database of Abe et al. (1990)

From the handbooks of Arctander (1969), which contain the semantic odor description of 3102 perfumery materials, Abe et al. (1990) discarded all mixtures and obtained the words describing the smell of 1573 compounds. In total, 34 terms were applied to 30 or more aroma chemicals. For two given descriptors (a and b), the authors calculated the overlap coefficient (c_{ov}) according to Eq. (1), being N_{ab} the total number of compounds described with both terms, while N_a and N_b is the total number of compounds labeled with attribute a and b, respectively:

$$c_{ov} = \frac{N_{ab}}{\min(N_a; N_b)} \cdot 100 \tag{1}$$

This coefficient is zero for descriptors that are never applied together and, conversely, the maximum value (100%) indicates that both terms appeared always simultaneously in the odor descriptions. The array containing c_{ov} coefficients for all possible pairs of the 34 descriptors is available (Table 2 of Abe et al., 1990). In this symmetric matrix, which will be referred to hereafter as S_{Abe}, the elements of the main diagonal are 100.

2.2. Olfactory database of Sigma–Aldrich (2003)

The Flavors and Fragrances Catalog of Sigma–Aldrich Fine Chemicals (SAFC) contains 881 ingredients (natural materials, aroma chemicals and mixtures) that are classified in 29 main odor categories (Sigma–Aldrich, 2003). Seven of them are subdivided into a different number of subcategories, which makes in total a pool of 82 odor descriptors (Zarzo & Stanton, 2006). A preliminary analysis suggested that terms with less than 13 occurrences do not provide reliable information for the purpose of the present study, and they were disregarded. The floral category comprises 15 descriptors, but 12 of them correspond to less than 13 ingredients. Thus, all materials listed under any floral subcategory were labeled as 'floral'. The same criterion was applied to materials under the fruity, citrusy and nutty categories. As a result, the final number of descriptors was 34.

By checking the terms assigned to each ingredient, the overlap coefficient (Eq. (1)) was computed for each pair of descriptors, which led to a similarity matrix (S_{SAFC}).

2.3. Multivariate statistical analysis

Principal component analysis (PCA) is a standard multivariate method. In most cases, the interpretation of results becomes more straightforward when the matrix columns are mean-centered prior to applying PCA. In this case, given that S_{Abe} and S_{SAFC} are symmetric arrays, they were double-centered using the procedure applied by Chastrette et al. (1991) (Eq. (2)), which leads to transformed matrices suitable for PCA (Gower, 1966) that will be referred to as T_{Abe} and T_{SAFC}, respectively:

$$t_{i,j} = c_{i,j} - c_i - c_j + c \tag{2}$$

where $t_{i,j}$ is each element of the double-centered matrix T; $c_{i,j}$ = element (overlap coefficient) of the similarity matrix S, c_i = mean of row i; c_j = mean of column j; c = mean of all elements of S. As a result of this transformation, the average of all rows and columns becomes zero. Next, PCA was applied using the software SIMCA-P 10.0 (www.umetrics.com). This procedure is equivalent to the multivariate method called Multidimensional Scaling (MDS) (Borg & Groenen, 2005), which is a standard technique for the analysis of similarity matrices.

In PCA, the contributions of variables (matrix columns) in the formation of a given component are called loadings, being $p[1]$ the loadings in the formation of the first principal component (PC1), and so on. In this case, the plot that depicts $p[2]$ vs. $p[1]$, which will be called PC1/PC2 loading plot, highlights the main similarities and dissimilarities among descriptors and it can be regarded as a 2-D sensory map of perfumery scents (Zarzo, 2008).

By visually inspecting the loading plots with different combinations of components, it was found that certain pairs of descriptors with a strong similarity exert an excessive contribution in the model. Thus, it was necessary to reduce their influence by applying weight coefficients, as further described below, which leads to a weighted matrix (W_{Abe} and W_{SAFC}). The resulting PC1/PC2 loading plots obtained by applying PCA to these matrices were visually inspected and compared.

2.4. Comparison with other sensory maps

The database of Boelens and Haring (1981) is a large compilation of numeric odor profiles. The data were obtained by a panel of six perfumers who smelled 309 aroma chemicals and rated the odor similarity on a 0–9 scale with respect to 30 standards commonly used in perfumery. Each standard was selected as a reference material for certain odor descriptor. This compilation, which will be referred to as B-H database, was analyzed using PCA in a previous study (Zarzo, 2008). The correlation between loadings of the B-H database with respect to those from the two databases studied here was checked in order to discuss if the underlying latent structures is basically the same.

The loading plots obtained provide valuable information to discuss fragrance wheels reported in the literature. One of them is the Discodor (Harder, 1979), which was developed by perfumers working at Haarmann & Reimer (Germany). It was also compared with the Fragrance Wheel of Edwards (2010), the Odor Effects Diagram (Calkin & Jellinek, 1994) and the Olfactory Spectrum (Kraft, Bajgrowicz, Denis, & Fráter, 2000). The Drom Fragrance Circle (reproduced by Jasper & Wagner, 2008) is another sensory wheel comprised by 16 categories, which were conveniently arranged to resemble as much as possible the other odor maps.

2.5. Interpretation of the underlying latent structures

PC1 of the B-H database discriminates refreshing (light) vs. warm (heavy) odors (Zarzo, 2008). Light scents are those that