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SketchOscent: towards a knowledge-based model and interactive visualisation of the odour space

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Abstract

The representation of an odour space is a challenging issue for scientists and professionals working in odour-related activities. Many food and non-food sectors have created their own classification system and representations of the odorant space to manage objective communication about odours. More generally, many representations of the odorant space have been proposed. These initiatives turn the odorant space into easy-to-digest representations classifying hierarchically a restricted set of odorants in specific categories that provide a common frame of reference to professionals or sensory analysis judges. Nevertheless, the odour set is often restricted and these representations do not reflect the continuum of current odours which are not frozen in single section but on the contrary closely overlap. Thus, the related visualisations face with difficulties to represent such odour relationships.

This work based on knowledge graphs from semantic web aims to propose a readable, interactive and publicly available representation of the aroma space, dedicated to olfactory and sensory practices. This representation relies on a large set of odours and takes into account overlapping categories.

The knowledge-based model thus produced includes about 380 odours which are distributed in 20 main categories, which are decomposed into 117 subcategories. Seventy-seven odours and 26 categories obviously belong to multiple categories depending either on the multidimensional perception they are suggesting or on a conceptual positioning. The odour space is fully encoded into an rdf/owl Knowledge Graph, a semantic web standard language, which can be easily edited, stored, shared and requested. A hierarchical visual representation is derived to get a friendly and readable representation. The flexibility introduced by this representation enables to easily find out the relevant term(s) needed to describe an odorant perception. This approach, applied to food application, can be expanded to non-food sectors such as odour environment for example. *SketchOscent* is freely and publicly available at <https://oniris-polytech.univ-nantes.io/sketchoscent>.

Keywords: odour space representation, human knowledge-based model, semantic representation, interactive visualisation, olfaction.

Introduction

The representation of an odour space is a challenging issue for scientists and professionals working in odour-related activities. Many food sectors such as coffee, whisky, tea or honey have created their own aroma wheels to exchange and communicate easily about odours.

Many representations of the odorant space have been tempted through the 20th century, mainly based on 3 approaches that rely on features of 1) the sensory organ, 2) the sensory stimulus and 3) the sensory percept [1, 2]. Considering the 320 odour receptor types discovered in humans, the first approach has been largely discarded to establish a simple odour classification based on relations between odour classes and receptor types. Similarly, if the chemical structure of an odorant strongly determines its perceived quality, all single measures have failed to predict or explain its odour perception. Thus, structure-odour relationships approaches failed to propose basic classifications. From the first model based on olfactory percepts proposed by Henning in 1916, many models have followed this approach, assuming that odours can be located in a n-dimensional space where their relative position reflects their similarity [1, 2]. However, the methods of analysis used to exploit the data sets are often inadequate to achieve a comprehensive and faithful projection of the odour space. As supposed by Chastrette [1], the olfactory space has probably a weak structure, a high dimensionality (with a signification of that dimensions that remains unclear), with classes of odours not sharply delineated. These outcomes should be linked to the subjective character of the data handled through the perception of the odorants, their conceptualisation and verbalisation [2]. Thus, none of the different models proposed elicit unanimity and the related visualisations face with difficulties to represent such odour relationships and fail to deserve more general fields of sensory practises.

Some works dealing with representation of the odour space, address the challenging issue of the visualisation of this odour space and of its categorisation/classification structure.

In their seminal work about the Field of Odour [3], Jaubert et al. (1995) proposed a visualisation map into a *half wheel* of 52 odours among 12 categories without hierarchy, resulting from the analysis of 1400 aroma

compounds. In the context of urban odours, *SensoryMap* [4] by McLean (2014) organised the odours into a bipartite graph with 2 wheels/rings: the inner ring enumerates 47 categories without hierarchy grouped into 4 families, and the outer ring 355 odours. Another wheel-based visualisation, *Flavor Network* [5], is introduced by Ahn et al. (2011) in order to achieve food pairing for cooking recipes. The visualisation is a single ring of 936 odours grouped into 34 categories without hierarchy. A pairwise relationship between odours is available from co-occurrence on the same compounds. The visualisation is interactive: when clicking on one odour in the ring, the edges with all the co-occurring odours are drawn. In the frame of perfume industry, Baud (2019) designed *ScentTree* [6], a tree like zooming visualisation composed of a hierarchy of 86 categories organised into 6 depth layers starting from 16 main categories, where 552 raw materials used in perfumery are categorised in tree leaves. The category hierarchy was built by a group of experts in fragrance. The visualisation is available online on the web but it offers a limited interactivity by zooming. Liu et al. (2019) visualise a hierarchy for odours with a *circular dendrogram* resulting from an AHC [7]. They limit the representation to 100 odours, and they show 9 main clusters for candidate categories to be identified.

Most of these visualisations are data based and use wheels of odours, where the odour set is restricted and without a detailed hierarchy, restricted to a single layer of categories. They are resulting from a data analysis for classification or clustering, and consist in static map drawings without interaction abilities, and their readability strongly decreases with the increasing of the number of odours. ScentTree approach is the most interesting for a meaningful odour space representation, because it delivers a hierarchical organisation of the odours into categories from the most general to the most specific based on human expertise, and it is available online on webpage interface. Unfortunately, it is very specific to perfume industry, the number of odours is restricted, it shows a readability issue due to a “lost in maze” effect when zooming in, and the interactivity is limited to zooming in/out.

In this context, this work aimed to propose *SketchOscent*, a new visual and interactive representation of the food-related odour space, dedicated to olfactory and sensory practices, relying on a large set of odours, that takes into account the continuous and overlapping nature of the odour space and in which odours can be described by different levels of accuracy and related to several odour categories considering either a perceptual or a conceptual approach. On the contrary of existing representations for classification/categorisation of odours which are mainly *data-based*, our approach proposes both a novel *human knowledge-based* representation in a *Knowledge Graph* delivered by domain expert working in odour-related field, and an adapted visualisation which is readable, interactive and publicly available.

Experimental

Data sources

Data from different sources were extracted and gathered to set up a list of odorant descriptors.

Among the numerous sources that catalogued description of odorant materials, we referred to the olfactory description of molecules referenced on “The good scents company” [8] and “Flavornet” [9] websites databases. These databases were selected owing to the accessibility of the data, their food or natural constituents relative content and a sufficiently high number of descriptors (872 and 197 respectively) referring to a large number of odorants (2360 and 660 respectively), which enable to consider a large spectrum of the food-related odour space. Quality description of odorants is obtained from the published literature on odorants detected by quantitative GC-O for the Flavornet dataset while it results from expert’s description for that found on The Good Scents Company dataset.

Modelling and conceptualisation

The process was challenged by domain experts in olfactive description and olfactometry. Their tasks consisted in firstly modelling a semantic hierarchy of categories/classes of odours (a partial order for generalisation/specialisation relationships between categories which are odorant descriptors as well), secondly the classification/categorisation of the odorant descriptors into the correct categories. These tasks were facilitated both by the list of all available odorant descriptors (vocabulary) and by a set of questionnaires for odour pairing to check the hierarchy and the overlapping of odours. These tasks resulted in a *Knowledge Graph* representation where the vertices are odorant descriptors and the arcs are the categorisation relationships between odorant descriptors. Technically, the representation is implemented in RDF semantic web language which can be easily edited, stored, requested and shared as linked open data.

Interactive visualisation

The representation of the odour space is based on 6 principles: (1) *completeness* - large amount of odours and relationships; (2) *meaningfulness* - human semantic map; (3) *structuration* - hierarchy of categories, odour pairwise relationships, (4) *readability* - wheel-based and hierarchical graph layout, mental map preservation, (5)

interactivity - abilities to browse, zoom, search in the visualisation, (6) *availability* - publicly available visualisation and embedded in a webpage, bilingual English/French, semantic web technology.

Results and discussion

Statistics

The knowledge-based model includes about 380 odours which are distributed in 20 main categories, which are decomposed into 117 subcategories partially ordered in a 6-level depth hierarchy with 644 “general to specific” relationships. Seventy-seven odours belong to more than one odour category, and 26 subcategories belong to multiple categories depending either on the multidimensional perception they are suggesting or on a perceptual or conceptual positioning.

Visualisation

A hierarchical visual representation is derived from that Knowledge Graph to get a friendly and readable representation (Figure 1). This representation consists in a circular/wheel-based and centripetal graph layout derived from the Yifan-Hu algorithm. It was generated on the basis of a minimal spanning tree topology and authorise odour duplication to reflect the belonging of odours to multiple categories. *Vertices* represent odours and can either stand for general odours (categories) or more specific odour (instances). The *text label* of vertices stands for the odorant descriptor either in French or English-speaking language. *Arcs* represent the oriented hierarchical relationships between odours (*i.e.* the covering relation of the partial order) and are oriented in a centripetal direction from the centre (more general) to the outer (more specific). *Colours* of vertices are associated to the depth level in the hierarchy. *Diameter* of Vertices is a log proportion of the number of instances belonging to each vertex.

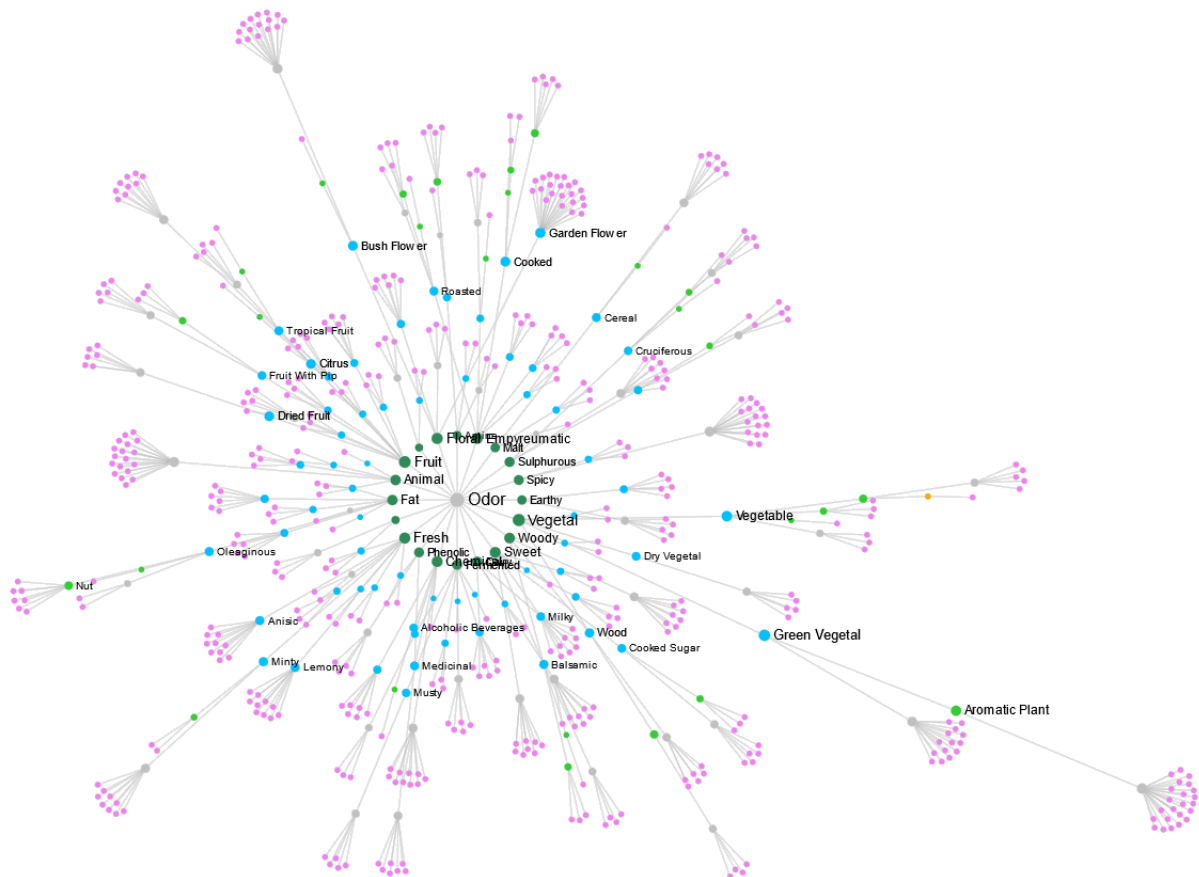


Figure 1: The SketchOscent, a hierarchical visual and interactive representation of the odour space derived from a knowledge-based model: global view.

Interactions

In addition to its graphical visualisation, the representation is endowed with interaction capabilities that allow the user to operate on it in order to facilitate information retrieval and local hierarchical relationships insight (Figure 2). We propose 5 operators: (1) Scaling for zooming in and out; (2) Searching for odours from text input; (3) Vertex Fly Over for highlighting the hierarchical neighbourhood of one vertex/odour; (4) Vertex Click On for

selecting and focusing on the partial subgraph of the hierarchical neighbourhood of one vertex/odour; and (5) Information for delivering more details about an odour/vertex such as more general odours, more specific ones, and a link toward the odours and raw materials in “The Good Scent Company” website. In all cases the global layout of the vertices is kept in order to preserve mental map of the user.

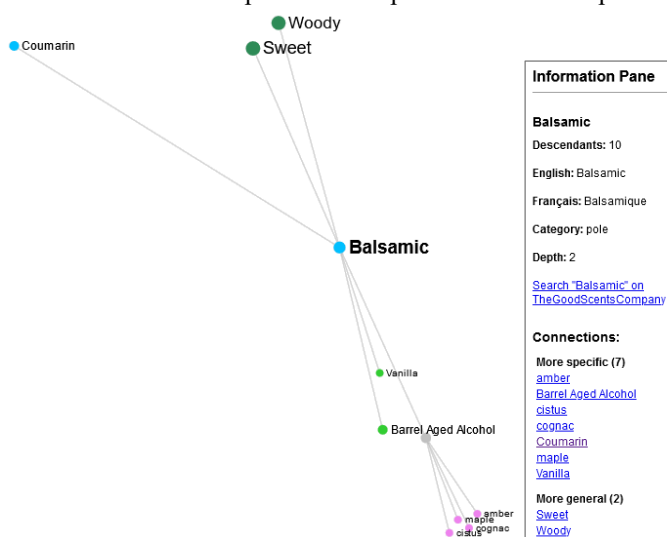


Figure 2: Local view of neighbourhood after clicking on the Balsamic vertex.

Conclusion

SketchOscent implements an original visual, interactive and hierarchical Knowledge Graph of the odour space founded on human domain knowledge. It meets the expectations of users for understanding and reasoning about odours and stretches boundaries of existing representations in terms of completeness, meaningfulness, structuration, readability, interactivity and availability. The flexibility introduced by this representation enables to easily find out the relevant term(s) needed to describe an odorant perception.

Perspectives for SketchOscent improvement consist in the possibility to extract partial subgraphs for food aroma subdomains (wine, cheese, meat, vegetables...), to change the colour assignment to show the root category belongings, mixtures and the overlapping of odours, or to display the relationships for co-occurrence of odours on same odorant materials.

This approach, applied to food application, can be expanded to non-food sectors such as odour environment for example.

SketchOscent is available at <https://oniris-polytech.univ-nantes.io/sketchoscent>

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