Quantifying Olfactory Perception: Mapping Olfactory Perception Space by using Multidimensional Scaling and Self-Organizing Maps

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Introduction

The role of higher cortical regions in olfactory perception is not very well understood. Scientists must choose their stimuli based largely on their personal experience. There is no guarantee that the chosen stimuli are able to span "olfactory perception space" appropriately.
A primary reason for that is there seems to be no known physical continuum for odor perception (akin to wavelengths of light for color perception). Hence it cannot even be assumed that there is a metric describing the olfactory perception space.
An olfactory perception database has been projected onto the nearest high-dimensional Euclidean space using a multidimensional scaling approach. This yields an independent Euclidean interpretation of odor perception, whether the space is metric or not. Self-organizing maps have been applied to produce two-dimensional maps of the Euclidean approximation of olfactory perception space.
This report will give a comprehensive look at the basic idea of this mapping approach and the application onto a psychophysical odor perception database.

Keywords: *Olfactory Perception, Multidimensional Scaling, Self-Organizing Maps*

Method

Published databases of smelling chemicals (odorants) like *Aldrich Flavor and Fragrances Catalog* **[1]** and Dravnieks *Atlas of Odor Character Profiles* **[5]** are focusing onlink chemical profiles with their evoked odors. Odorants (e.g. *Hexyl Butyrate*) are characterized by complex patterns of odor descriptors (e.g. *fruity, sweet, pineapple*). Data matrices may be developed from this information and used to extract odor similarity information by analyzing the transposed matrix **[3]**. Although the search for an odor descriptor basis is not over yet, such odor characterizations have been shown to be stable **[4]**.
A dataset based on *Aldrich Fragrances Catalog* (including 851 chemicals using 278 odor descriptors) has been used for a first mapping approach by Chee-Ruiter in 2000 **[3]**. We will refer in the following to the same database as a source of information for our sketch of the odor space.

For estimating dissimilarities between different odors intuitively most satisfying results have been obtained using the subdimensional distance d_s. This dissimilarity measurement is defined as

$$d_s(O_x, O_y) = \frac{\sum_{i=1}^{n} \left| o_i^x - o_i^y \right| \cdot o_i^x + \frac{\sum_{i=1}^{n} \left| o_i^x - o_i^y \right| \cdot o_i^y}{\sum_{i=1}^{n} o_i^y}}{\sum_{i=1}^{n} o_i^x + 1}$$

with $O_x = (o_1^x, ..., o_n^x)$ and $O_y = (o_1^y, ..., o_n^y)$ two observation vectors.

Information for a reasonable map has been extracted from a *(278x278)* odor dissimilarity matrix by Multidimensional Scaling (MDS). As a branch of multivariate data analysis MDS identifies important dimensions of a given dissimilarity matrix. These dissimilarities do not have to be metric, because MDS is used to project the dissimilarities to the nearest Euclidean space. MDS is a common method for dimensional reduction and graphical representation of multidimensional data. Fortunately it can be used to estimate the dimensionality of a data set as well **[8]**.

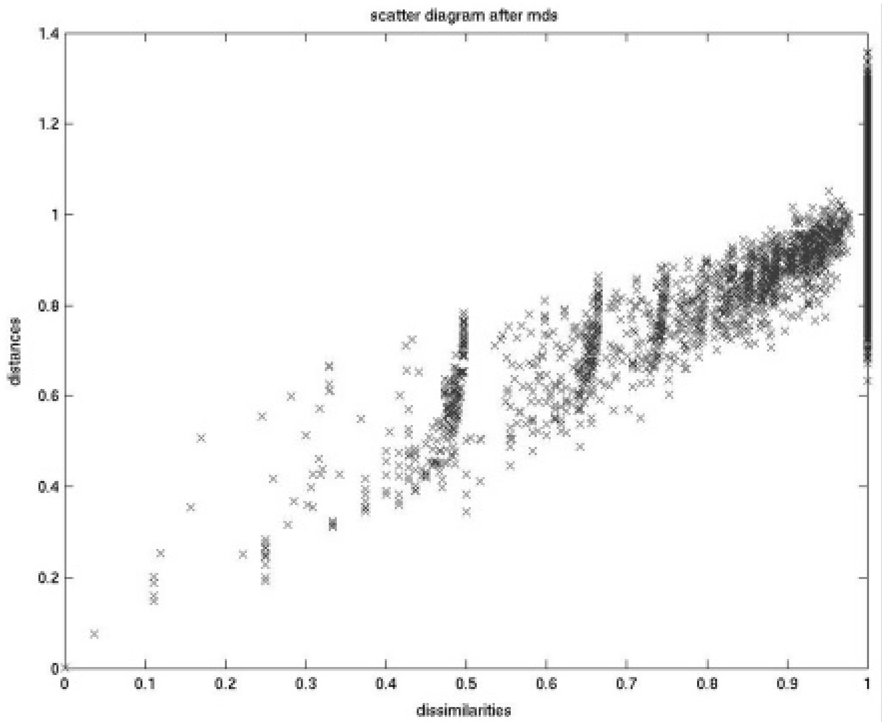

Figure 1: Scatter diagram after performing 32 dimensional multidimensional scaling on similarity matrix based on Aldrich database. The d_s dissimilarities are plotted against the estimated distances after MDS.

Application of a slightly modified MDS to the odor dissimilarity matrix resulted in a 32 dimensional Euclidean approximation of odor perception space. In **Figure 1** the original dissimilarities x are plotted against their Euclidean distance approximation y. A perfect projection would lead to $f(x)=y$. MDS on high dimension does not increase the projection's quality.

A self-organizing map (SOM or Kohonen map) is a set of artificial neurons, organized on a regular two-dimensional grid. With each neuron n_i a d-dimensional vector m_i is associated, where d is the dimension of input values. The neurons are connected to their topographical neighbours in the low-dimensional grid. These maps are able to learn the d-dimensional structure of a given input set without losing their low-dimensional order. That way complex structures can be analyzed and displayed in lower dimensions.

Results

We used a standard self-organizing map as introduced by Kohonen in **[7]** to learn about the structure of odor perception space. Its shape has been chosen to be toroid to be as flexible as possible in approximating a potential non-metric structure. The low-dimensional map is deformed while learning a high-dimensional structure, which leads to cases where high-dimensional neighbours are seperated on the low-dimensional map.

Figure 2 shows the resulting map. Clusters have been found by k-mean clustering **[6]**. The map has a toroid shape and because of the rough dimensional reduction the map shows formation of fragmented clusters.
This fragmentation persists in the labeled map as shown in **Figure 3** (e.g. celery, caraway and pleasant are embedded in fragmented cluster *15*, thus they are adjoining). Each odor descriptor has been plotted onto its best matching neuron on the map.

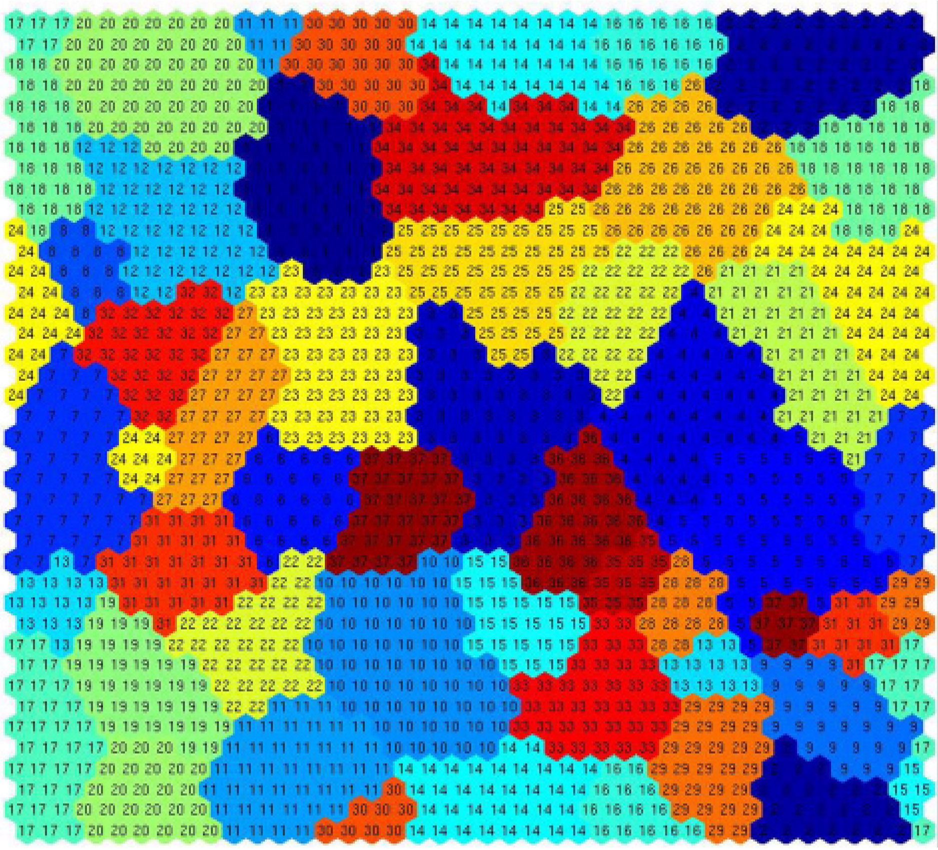

Figure 2: Odor perception map, clustered by k-means clustering. The self-organizing map has been trained on the 32 dimensional MDS approximation of the database. The surface of this Kohonen map is doughnut-shaped, thus some clusters are fragmented (e.g. cluster 15 located in the lower right corner and right below the center). Each neuron has been labeled with the number of its enclosing cluster.

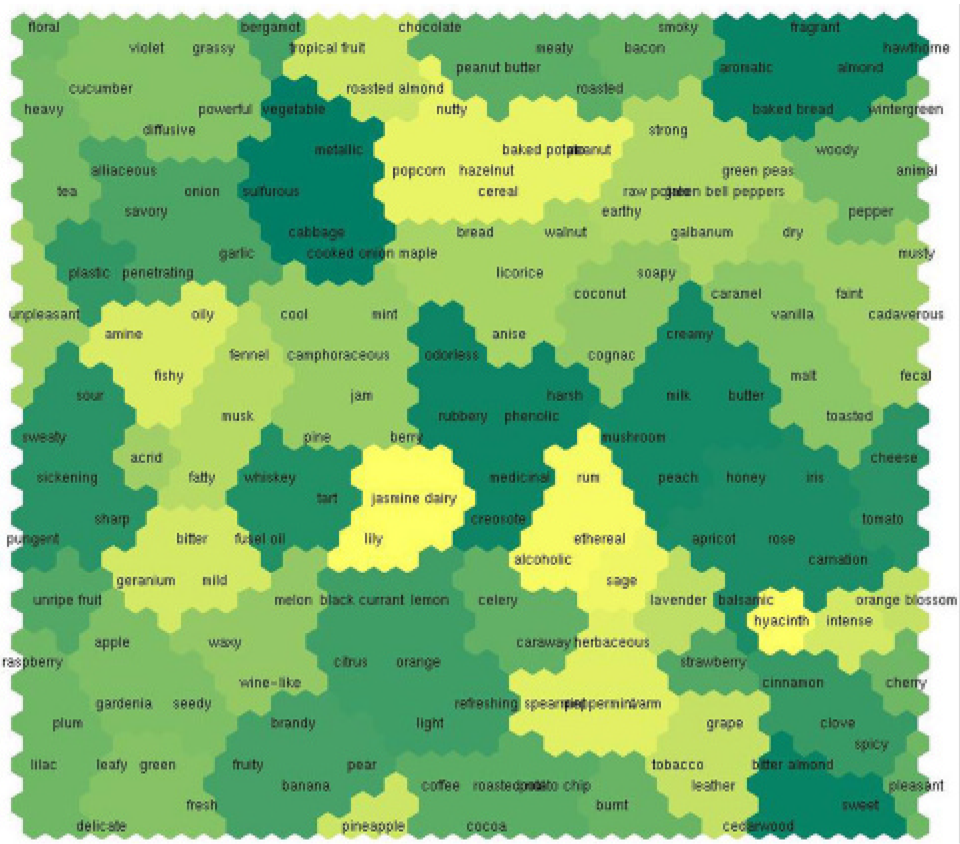

Figure 3: Odor perception map, labeled with odor descriptors. Each descriptor has been plotted onto its nearest neighbour on the SOM. The colored areas are the clusters corresponding to **Figure 2**.

Conclusion

We have expressed relationships between odors through a solid low-dimensional map. The presented infrastructure enables us to improve, extend and test the map in accordance to new odor data of any kind.
Thus this map will help to illustrate and to test hypotheses about the perception of odors.
For example, if all odorant compounds containing Nitrogen are processed similarly by the olfactory system, one would expect that only a certain set of odors will be evoked by them. If such a classification were a significant distinctive mark, this set of odors should not fall in random locations on the map.

The approximation via MDS strongly suggests that the odor perception space is high dimensional. The complexity of this space should be estimated in more detail, especially the meaning and number of this dimensionality.

Literature

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