PhD thesis position (CIFRE) in machine learning and analytical chemistry

Title: Perfumes comparison by combination of machine learning and analytical chemistry
Keywords: Perfumery, Olfaction, Odor additivity, Artificial Intelligence, Analytical Chemistry
Approaches: Machine learning, Deep learning, Cheminformatics, Gas Chromatography – Mass Spectrometry
Starting date: January 2022
Location:
- Université Côte d'Azur, Institut de Chimie de Nice, UMR 7272 CNRS, 06100 Nice (Fr)
- Perfumist, InnovaGrasse, Espace Jacques Louis Lions, 06130 Grasse (Fr)

Scientific description:
The brain is the most complex organ in the body. Its billions of neurons make specific connections according to their genetic programs and neuronal activities. Among the external signals, odors are arguably the most complex. The sense of smell is a powerful sense that can trigger intense emotion, stereotyped behaviors and lasting memories that cannot be accessed by any other sense. Decoding the psychological dimensions of odor perception has long been a central issue in olfactory research. Scientists working on olfaction as well as perfumery professionals have tried to establish standards for the description, measurement, and prediction of the quality of odors. Several odor classification systems have been developed in recent decades but remain incomplete to explain factors related to the organization of our olfactory system and to the inter-individual differences in the perceptual and verbal capacities of the subjects.

Perfumes are complex mixtures made of numerous ingredients that differ in their chemical structure, perception threshold, and relative concentration. An odorant molecule, even at very low concentration, may have a strong impact on the perceived odor/flavor and mask the other molecules of the blend, and thus the perceptual properties cannot be directly explained from the structure of individual molecules. The study of its constituents is then essential to describe the perfume as a whole. Perfumist is the number one mobile app designed to rank a selection of perfumes you are most likely to love with an ever-growing database of nearly 40k perfumes from over 1500 different brands. From the reference of a known perfume in its database, Perfumist applies an olfactory correlation algorithm in order to offer the best matches among thousands of existing perfumes on the market. The objective of the project is to mine the data describing complex molecular matrices to develop new similarity metrics based on artificial intelligence models. The first part of the project will be dedicated to setup a molecular database of perfumes obtained from analytical chemistry experiments. In a second step, the database will feed machine learning, as well as deep learning, models designed to predict the similarity between two perfumes. The last part of the project will be dedicated to deploying a new release of the Perfumist algorithm based on this new metric.

Candidate Profile: Master of Science degree or equivalent, strong background in physico-chemistry or computer sciences with skills in analytical chemistry (GC-MS) and machine learning. Knowledge in flavor and fragrances is a plus but not mandatory. Experience with python programming is required.

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