Machine learning for odor molecules psychophysiological effect prediction

Every day we are confronted with odorous stimulations. Beyond the natural smells that surround us, we make use of perfumes, deodorants or shampoos to modify our body odors. Furthermore, our clothes are impregnated by the fragrance of detergents or fabric softeners. Smells affect us on a physical, psychological and social level, and most of the time unconsciously.

Recently, machine learning models were developed to predict human olfactory perception qualities from chemical feature to some extent [1]. A crowd-funded challenge called the DREAM olfaction prediction challenge resulted in the development of several models which used machine learning algorithms that could accurately predict the pleasantness and intensity of molecules, as well as 8 out of 19 semantic descriptors (garlic, fish, sweet, fruit, burnt, spices, flower, sour,) [2]. However, to our knowledge, no model is available to predict the psychophysiological effect of odor molecules.

The particular neuroanatomy link between olfaction and emotion suggests that odors could evoke emotion and autonomic state [6]. Furthermore, many studies have suggested that the olfactory stimulation of fragrances or odor molecules produces immediate changes in physiological parameters such as temperature, skin conductance, heartbeat rate variation and respiration rate [3-5].

In this work, we presented a proof of concept that machine learning can be used to classify the odor molecules as enhancing activity (or positive effect "+") or a decreasing activity (negative effect "-") for heartbeat rate variation, temperature, skin conductance, and respiration rate. Such an approach will be of interest because it should allow to design and optimize odorants or perfumes to positively affect our emotional state.

Given the small size of our data set, (47 odor molecules with 524 features spaces), Support Vector Machine(SVM) algorithm and principal component analysis for dimension reduction were used to build a machine learning model for each physiological parameter. The different SVM models for the heartbeat rate, temperature, skin conductance, and respiration rate, achieved respectively an accuracy of 80%,90%,70%,60%.

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