Which Odorant Properties Are Most Relevant to Perception?

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Summary

The relationship between physicochemical properties of odor molecules and perceived odor quality is arguably one of the most important issues in olfaction and the rules governing this relationship remain unknown. Any given odor molecule will stimulate more than one type of receptor in the nose, perhaps hundreds, and this stimulation reflects itself in the neural code of the olfactory nervous system. Using archival data from animal psychophysics we investigate neural coding at the level of the olfactory bulb, the first relay for olfactory processing in the brain. Our results give insights into relevance of odorant properties to perception.

- Animals recognize a very high number of different odors and this is crucial in social interaction, feeding, and mating, as well as for the processes of learning and memory.
- There seem to be no apparent molecular features of the odorant that directly determine perceptive quality[3].
- In the rat nose there are 1000 receptor types[1], each of which corresponds to a combination of molecular features of the odorants[2].
- In the olfactory bulb, each glomerulus, bundles information corresponding to one receptor type.
- Which odorant properties affect the representations at the olfactory bulb most?
- Classification of each particular property from activations of glomeruli gives a measure of the property's relevance to perception.

- Experimental data by Leon group, UCI[4]
- Each rat was exposed to a particular odorant.
- They imaged 2DG uptake in rat olfactory bulb.
- Activation maps: 308 images · 1800 pixels.
- For each image we have a list of chemical properties and hedonistic descriptors corresponding to odorant.

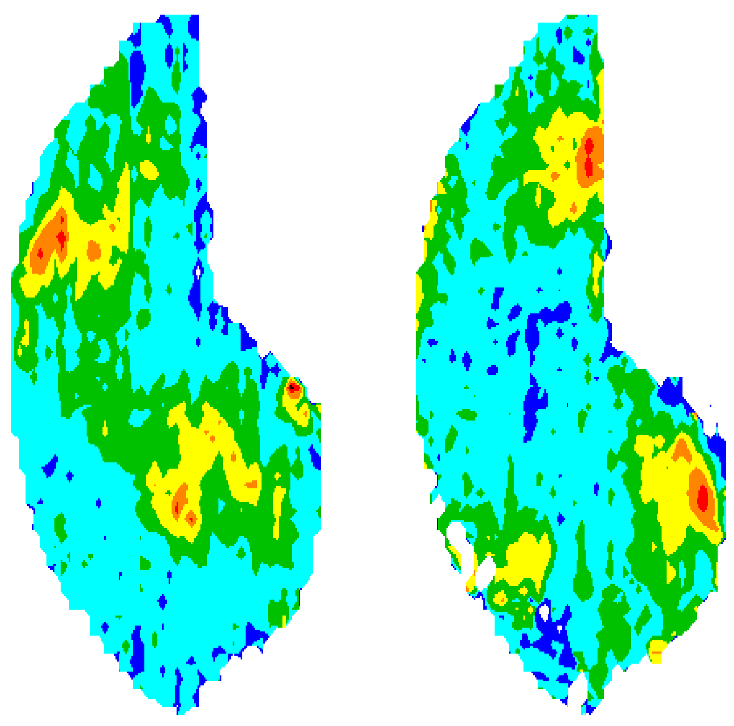

Figure 1: Glomerular responses to octanol (left) and propanol (right).

- Classification from activations within glomeruli to each property.
- Linear support vector machine (SVM).
- For each property, half of the maps were training and half test.
- We took all points as input vector and the property as target.
- We took the area under the receiver–operating characterics (AUC).
- 250 random subsamples.

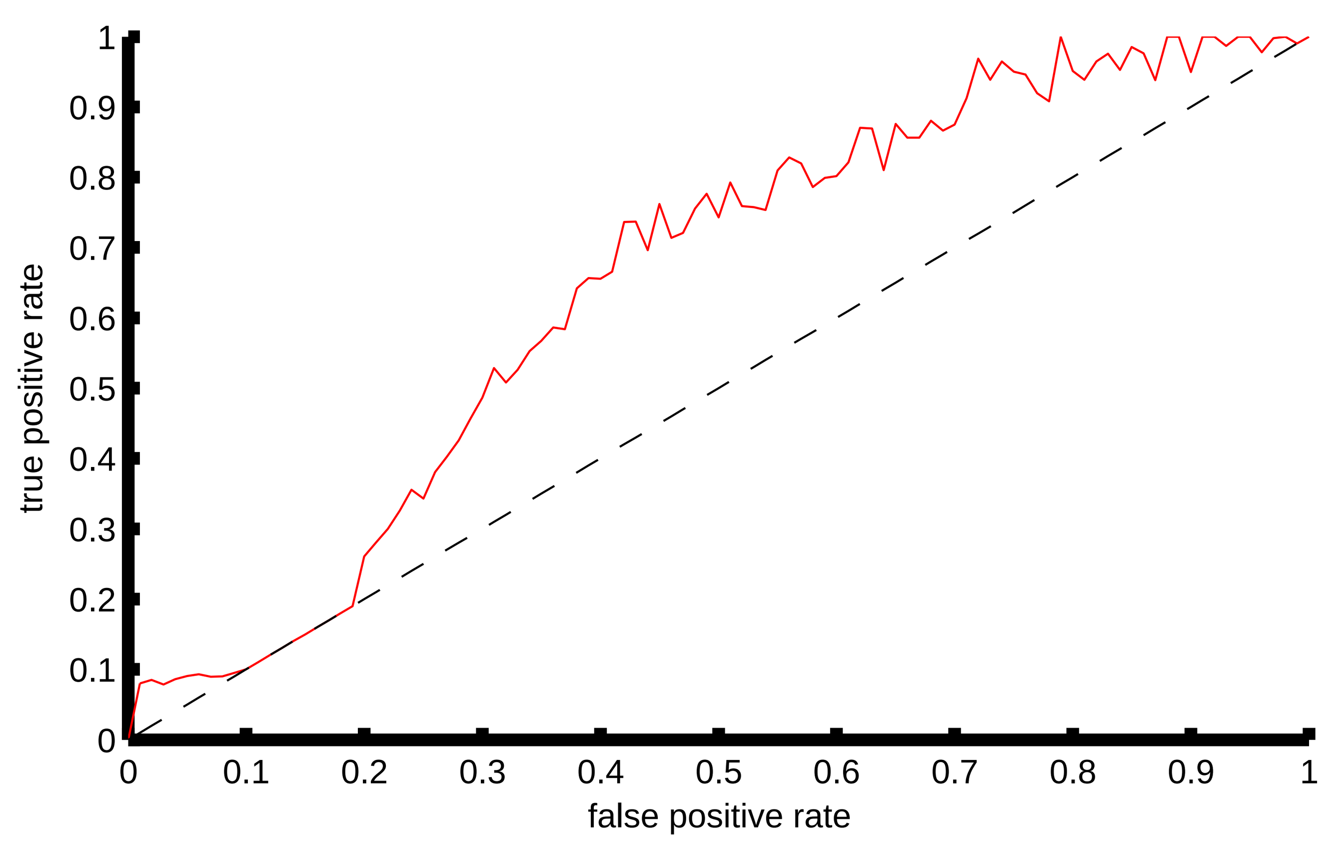

Figure 2: Illustration of a ROC Analysis

Classification Performance

We rank properties according to their classification performance (AUC).

odorant	AUC
sulfur–containing compound	0.99
alkyne	0.99
alkene	0.99
alkane	0.99
carboxylic acid	0.93
aromatic	0.85
ketone	0.78
ester+lactone	0.75
alcohol+phenol	0.73
alicyclic	0.70
heterocyclic	0.65
polycyclic	0.65
amine	0.50

- Sulfur–containing compound, akyne, alkane, and alkene performed close to ceiling.
- Carboxylic acid and aromatic also performed quite good.
- Ketone and ester–lactone, functional groups, and cyclization properties alicyclic, heterocyclic, polycyclic showed mediocre performances.
- Amine was worst of the compared properties, performing only at chance level.

- Some properties affect odor coding very strongly (sulfur–containing functional group).
- Bond saturation affects also seems very relevant (alkyne, alkane, and alkene).
- Carboxylic acid and aromatic, still seems to be important.
- Results partly confirm Johnson and Leon's important dimensions of molecular properties[5] cyclization, carbon numbers, bond saturation, branching, functional groups, and substitution position.
- Results partly confirm Yoshida and Mori[6] who proposed 14 primary odorant categories.

The authors thank Miquel Tarzan for implementing a support vector machine that was robust enough to make this study possible. One of the authors, B.A., is supported by a grant from the federal state government of Catalonia (formaciò de personal investigador, FI).

1. L. Buck and R. Axel. A novel multigene family may encode odorant receptors: a molecular basis for odor recognition. *Cell*, 65(1):175–187, 1991.
2. K. Mori and G. Shepherd. Emerging principles of molecular signal processing by mitral/tufted cells in the olfactory bulb. *Semin Cell Biol*, 5(1):65–74, 1994.
3. C. Sell. On the unpredictability of odor. *Angewandte Chemie International Edition*, 45(38), 2006.
4. B. Johnson, Z. Xu, P. Pancoast, J. Kwok, J. Ong, and M. Leon. Differential specificity in the glomerular response profiles for alicyclic, bicyclic and heterocyclic odorants. *The Journal of comparative neurology*, 499(1):1, 2006.
5. B. Johnson and M. Leon. Chemotopic odorant coding in a mammalian olfactory system. *The Journal of comparative neurology*, 503(1):1, 2007.
6. I. Yoshida and K. Mori. Odorant Category Profile Selectivity of Olfactory Cortex Neurons. *Journal of Neuroscience*, 27(34):9105, 2007.