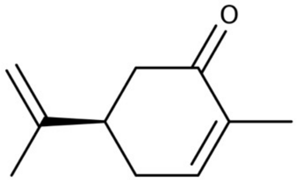

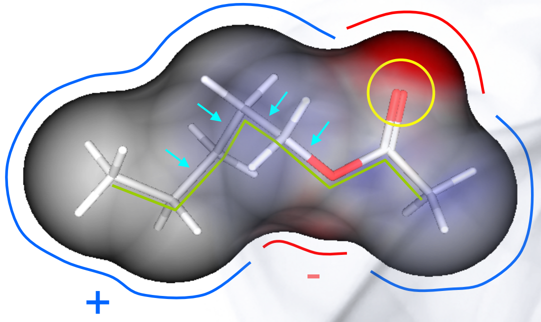

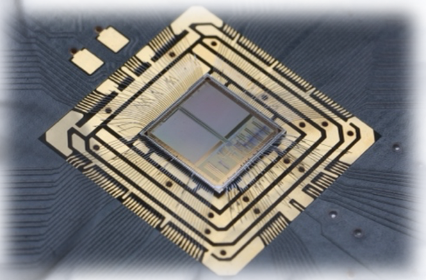

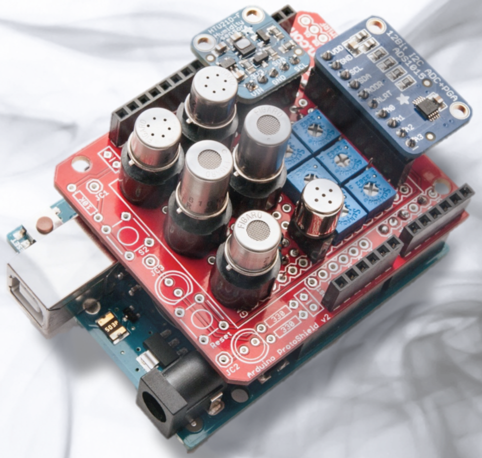

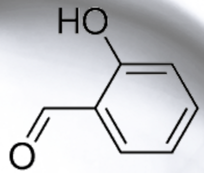

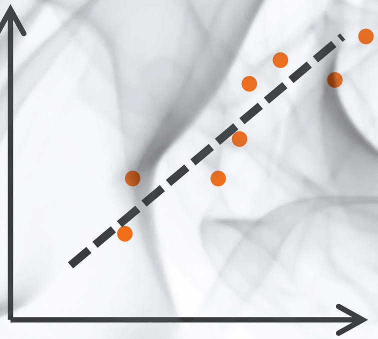

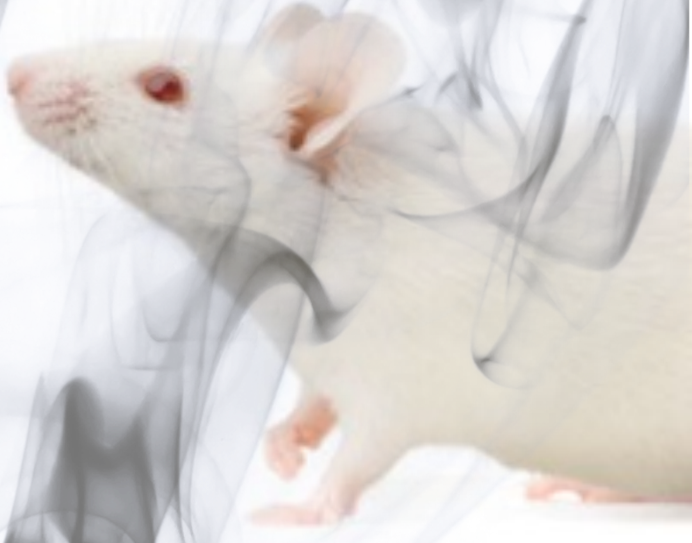

Odor spaces — From Biological Olfaction to Electronic Noses and Back Again

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http://biomachinelearning.net

nanoSeminar 25/11/2021
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Duke


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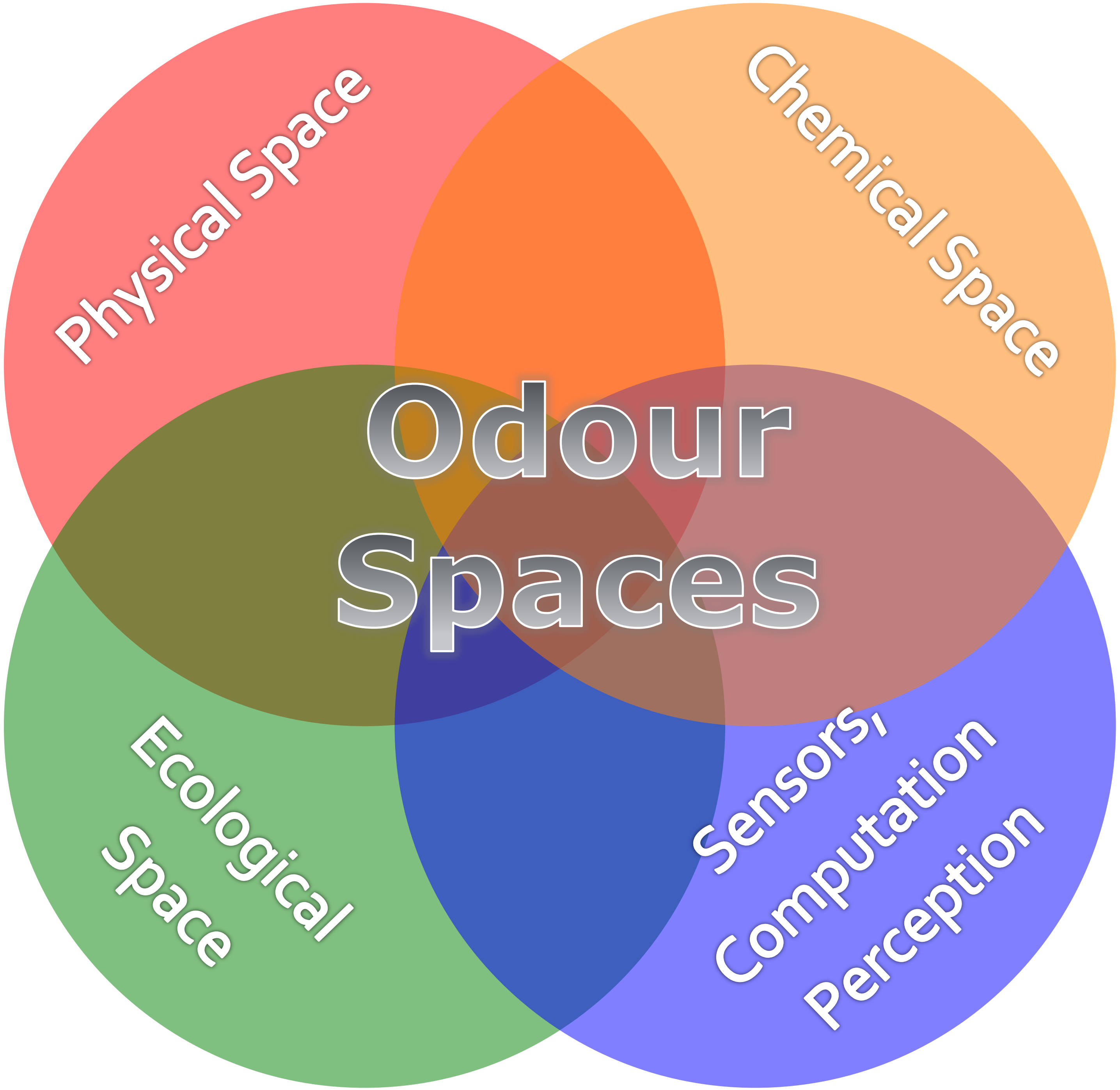
NeuroNex

ODOR2ACTION

https://odor2action.org

Funded by: NSF, MRC Medical Research Council, Thematic network supported by Fonds de recherche Santé Québec

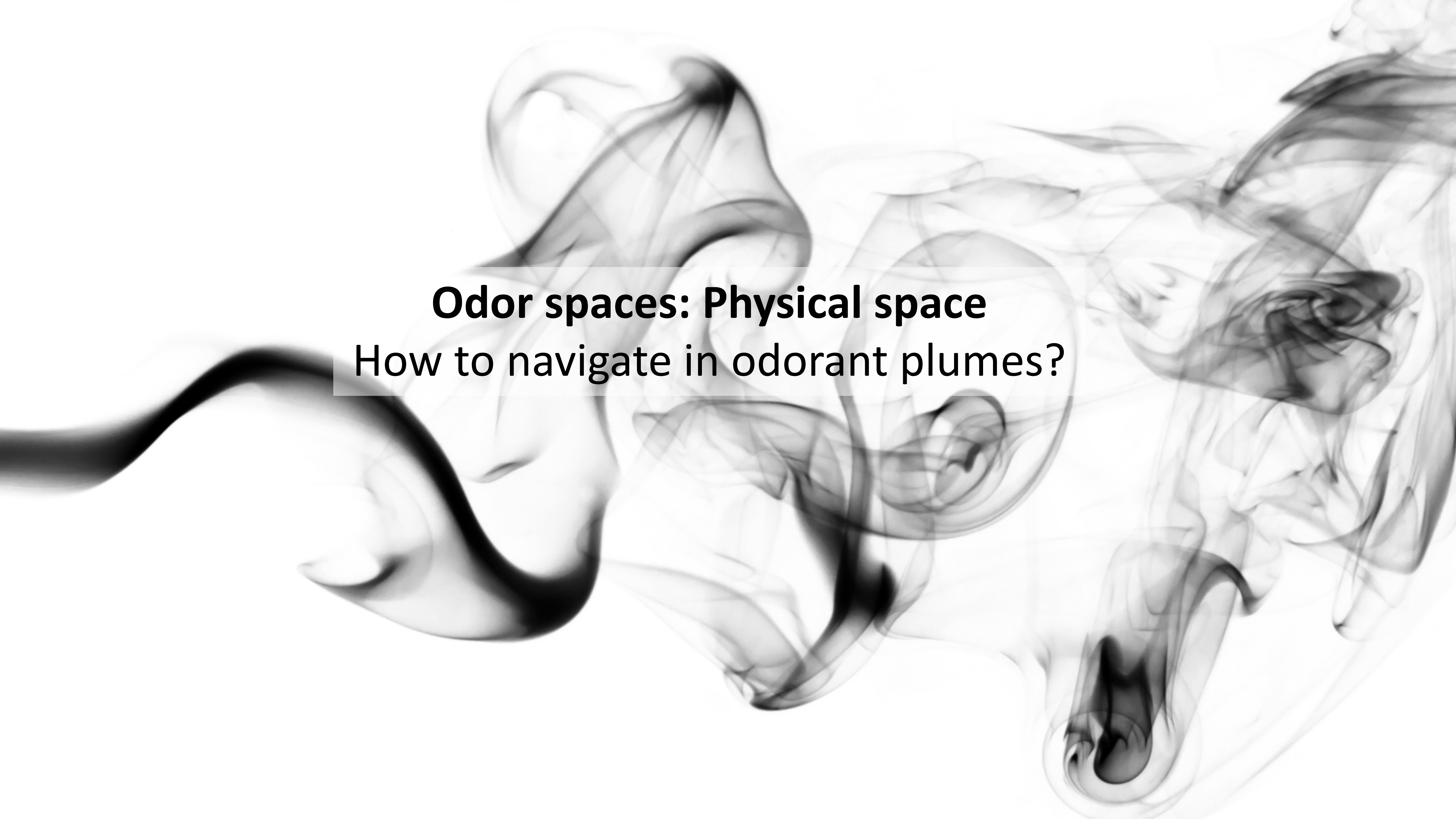


Aspects of “Odour Space”:

- Physical space: odour filaments in turbulent airflow.
- Chemical space: odorants.
- Sensors, Computation, Perception:
    - receptors and receptive fields.
    - neural computation for odour identification
    - hedonic odour quality
    - sensory integration and context-dependent odour
- Ecological space: Chemical ecology.

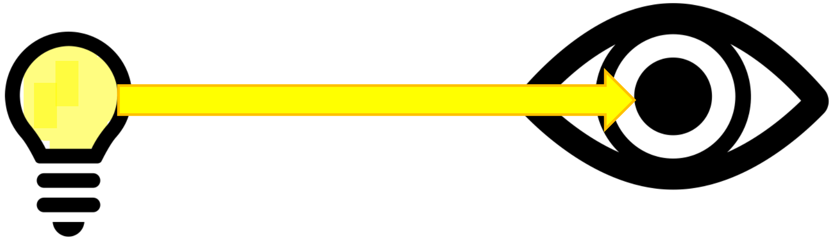
Odor spaces: Physical space

How to navigate in odorant plumes?

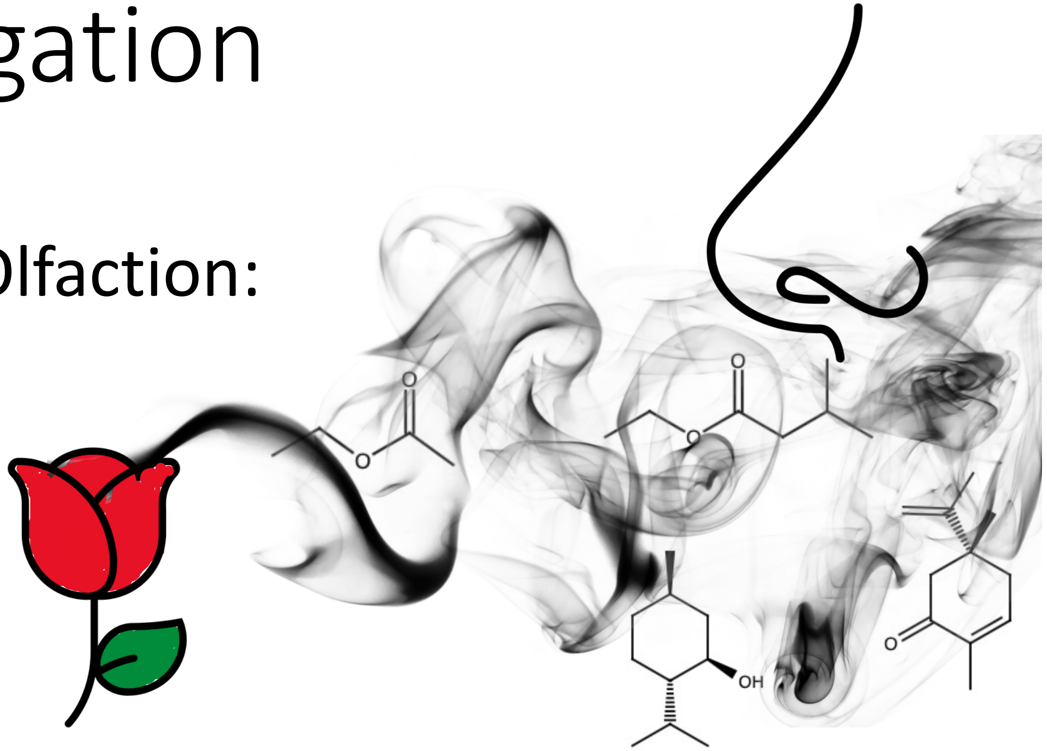


Stimulus propagation

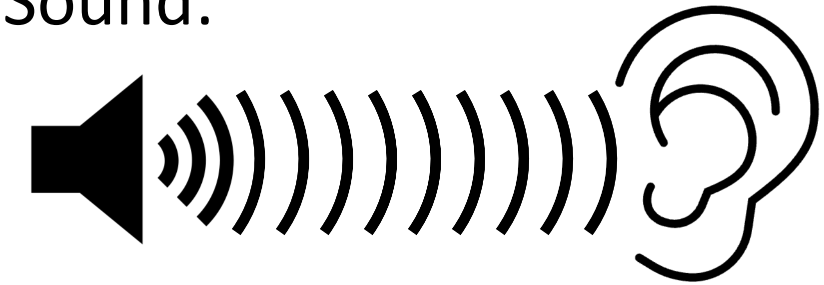
Vision:



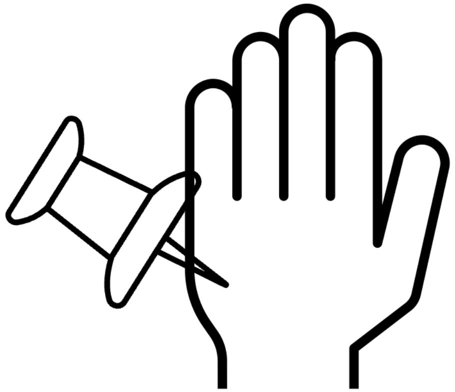
Olfaction:

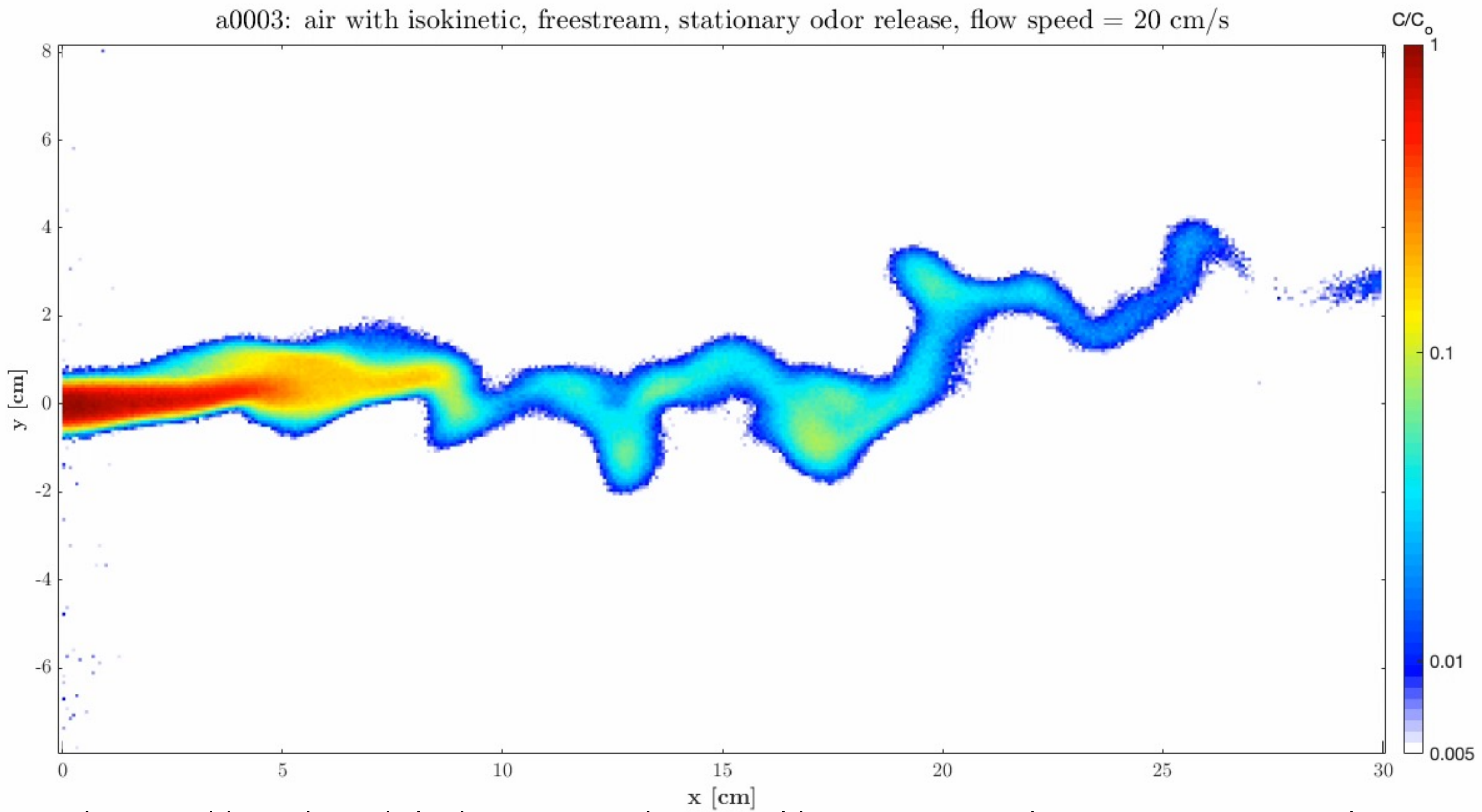


Sound:



Touch:





Courtesy John Crimaldi, Ecological Fluid Dynamics Lab, CU Boulder; NeuroNex Odor to Action NSF Award #2014217

NATURE
NATURE VOL. 303 30 JUNE 1983

Finding of a sex pheromone source by gypsy moths released in the field

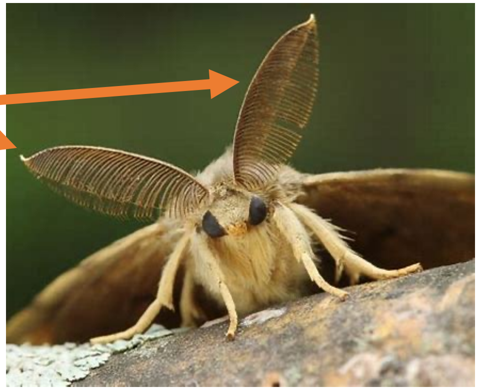
C. T. David*, J. S. Kennedy & A. R. Ludlow

Lymantria dispar L.

female

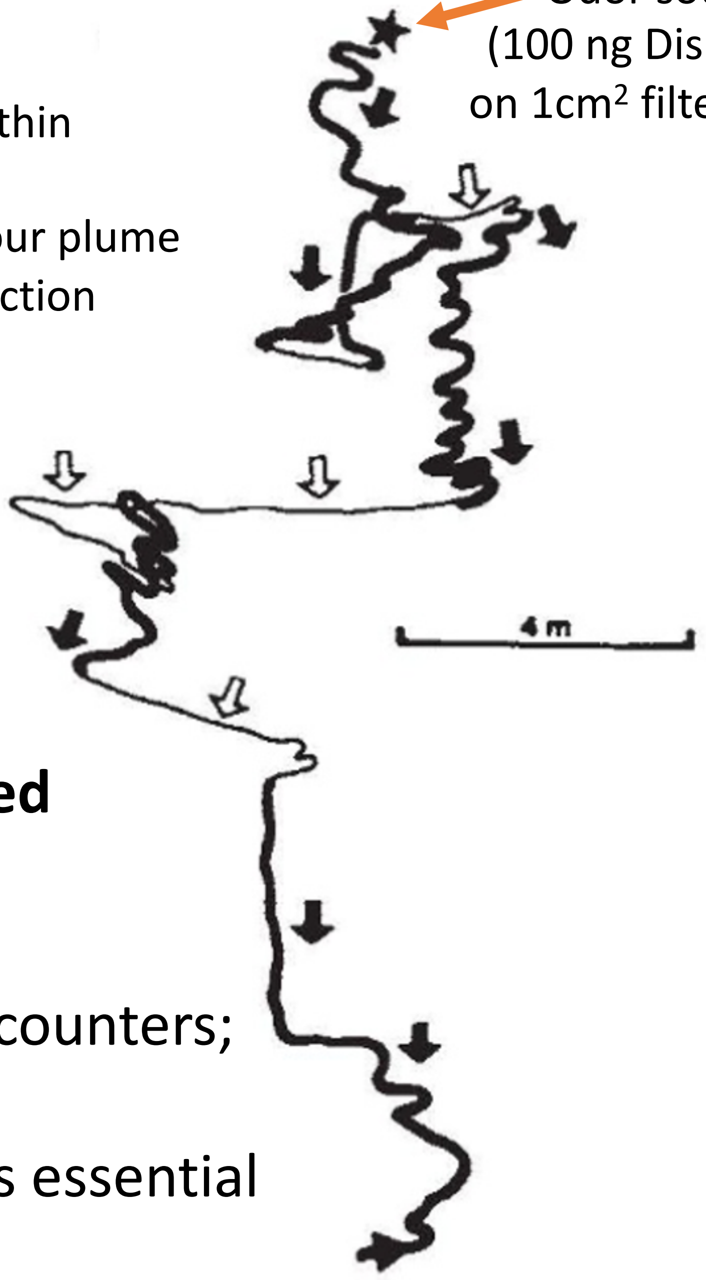
male

male antennae



Thick trace: Moth is within odour plume
Thin trace: outside odour plume
Arrows: local wind direction

Odor source (100 ng Disparlure on 1cm^2 filter paper)



General wind direction

“odour-modulated anemotaxis:”

Fly upwind upon odour encounters;
Fly crosswind otherwise.
-> **Low-latency detection** is essential

Two sources

flow

Spatial resolution ≈ temporal resolution

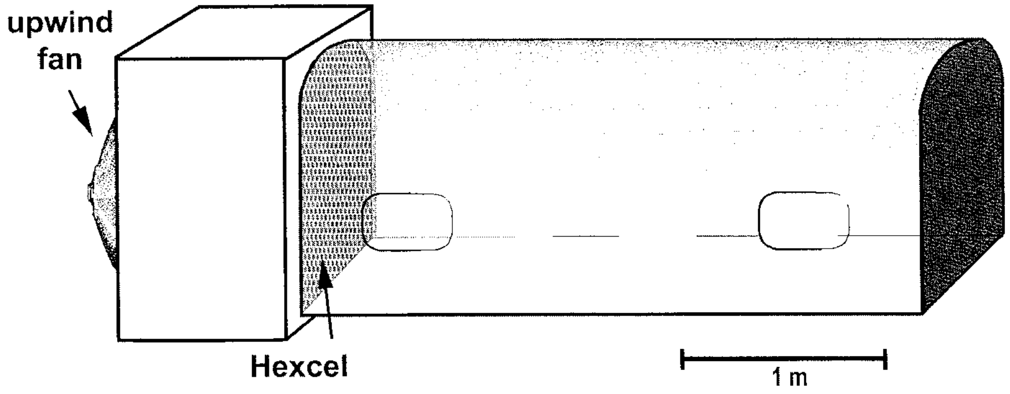
See also Hopfield, J. J. Olfactory computation and object perception. *Proc National Acad Sci* **88**, 6462–6466 (1991).

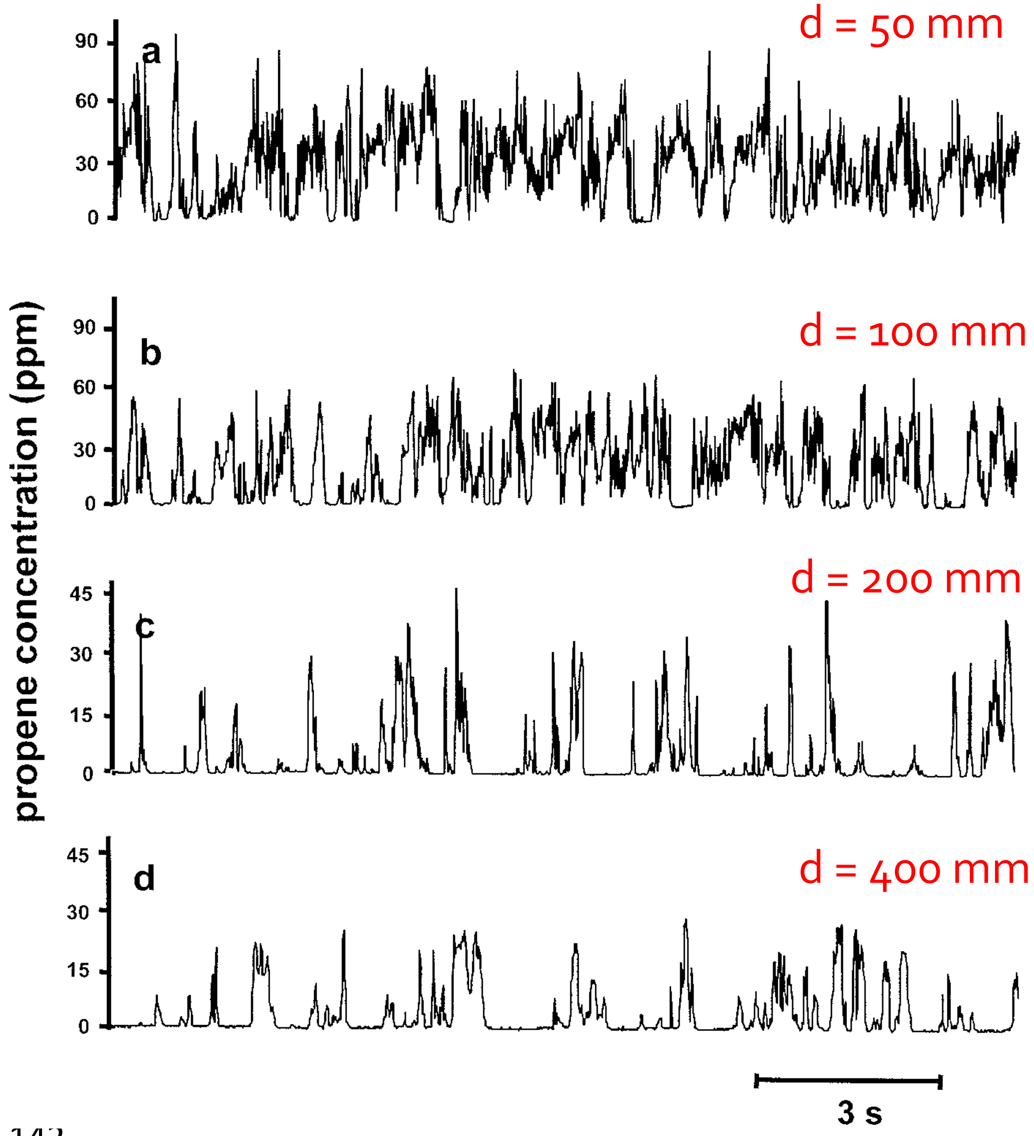
Plume image source: Celani et al. Odor Landscapes in Turbulent Environments. Physical Review X 2014.

Intermittency vs. distance in a wind tunnel

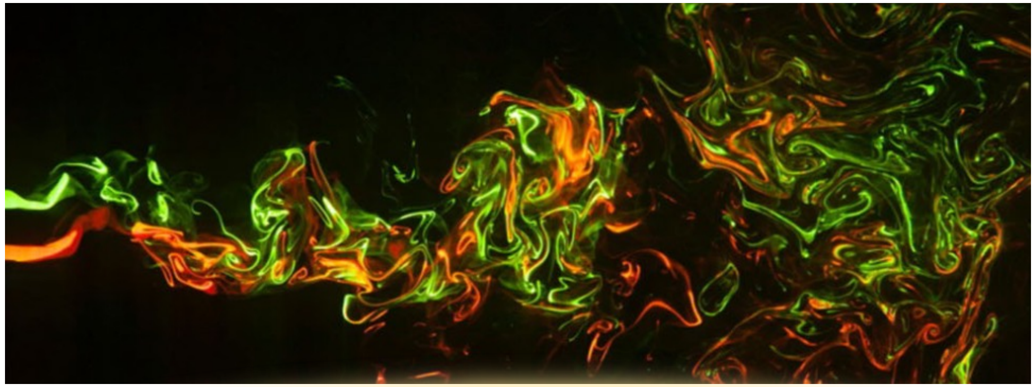
Wind tunnel experiments:

- Most salient difference is the change in intermittency.
- Max. concentration is also affected.
- Average concentration would be influenced by both factors.





Justus, K. A., Murlis, J., Jones, C., and Cardé, R. T. (2002). *Environ. Fluid Mech.* 2, 115–142.

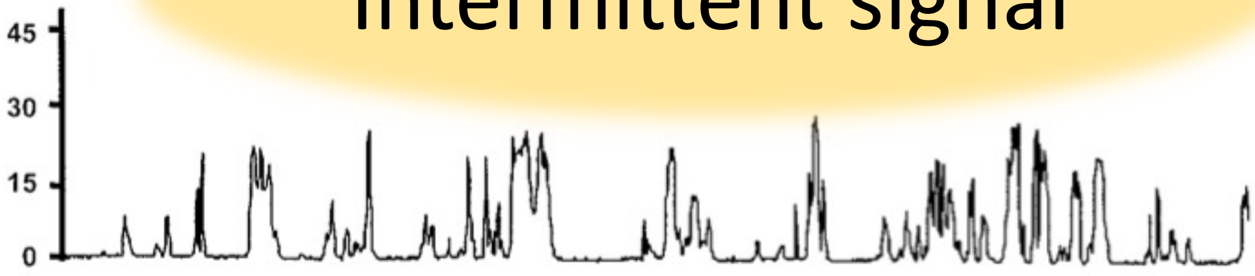


Low latency

High temporal resolution
& gas discrimination

The ideal sensor?

Intermittent signal



Gas sensing technology

Gas chromatography + Mass spectrometry (GC-MS), or Proton transfer reaction (PTR-MS)

- Precise gas recognition
- Bulky & power hungry
- Slow (GC-MS)

Photo-ionisation detection (PID)

- Fast but weak discrimination

Polymer Sensors

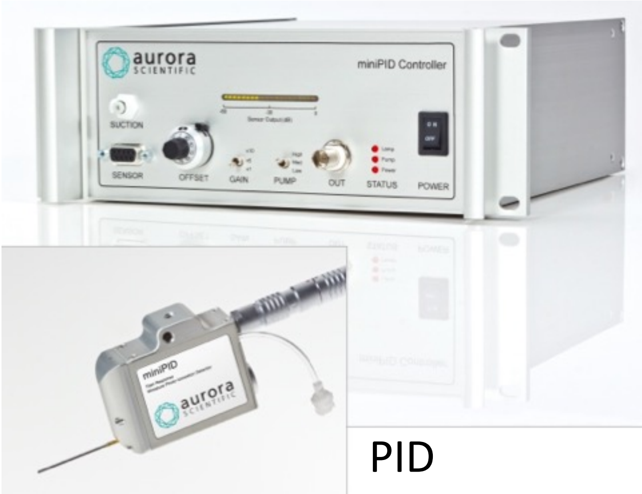
- Tunable to many compounds but require lab

Metal-oxide sensors (MOX)

- Good gas discrimination
- Small & commercially available
- Slow
  - But, hang on….

GC-MS

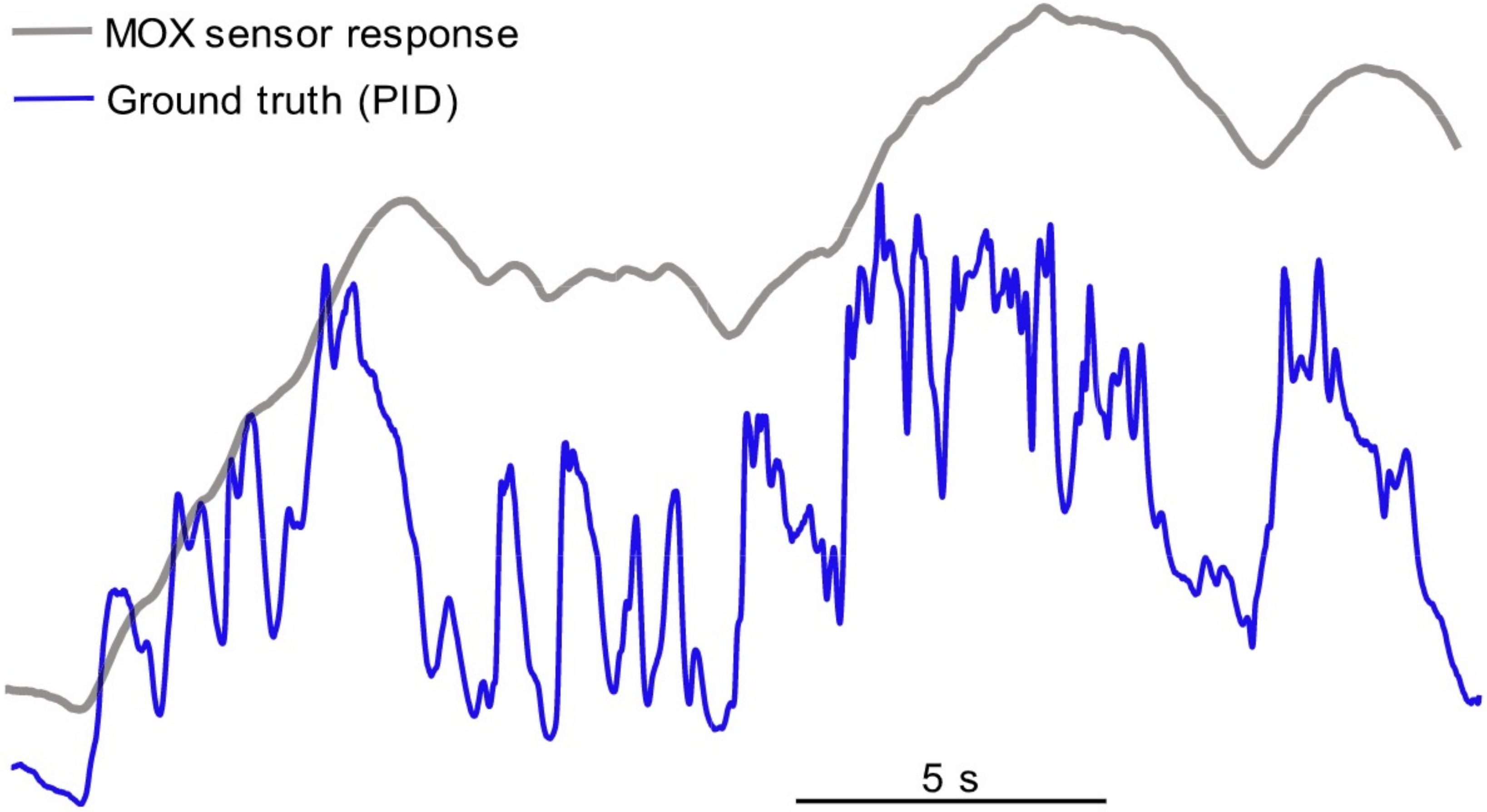
PTR-MS



PID

MOX

Practical issue: Slow recovery of MOx sensors



MOx trace is a low-pass/integrated version of true gas concentration.

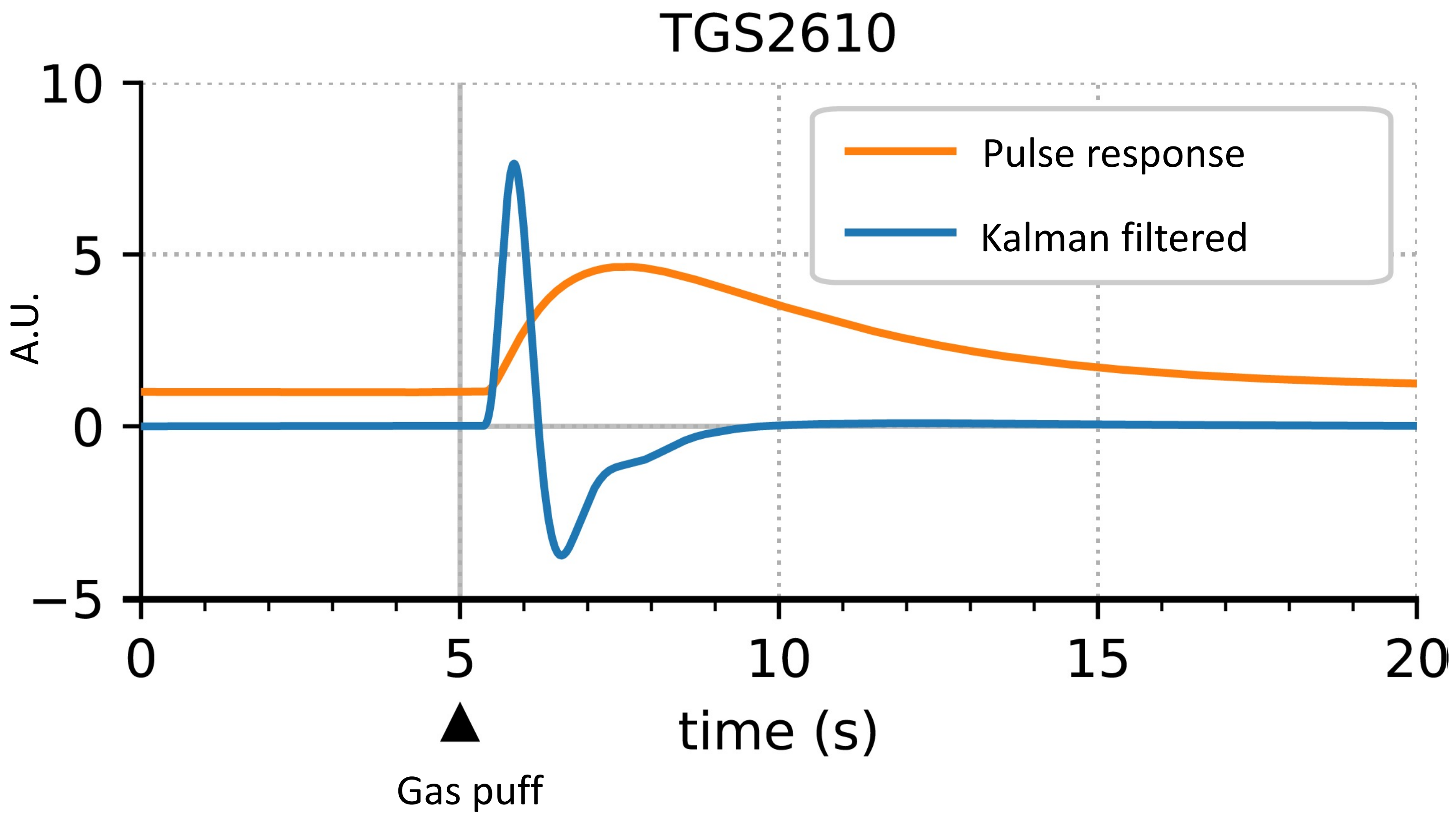
PID: Photo-ionisation detector.

Very fast, but cannot discriminate gases well.

Burgues & Marco, IEEE Access, 2020.

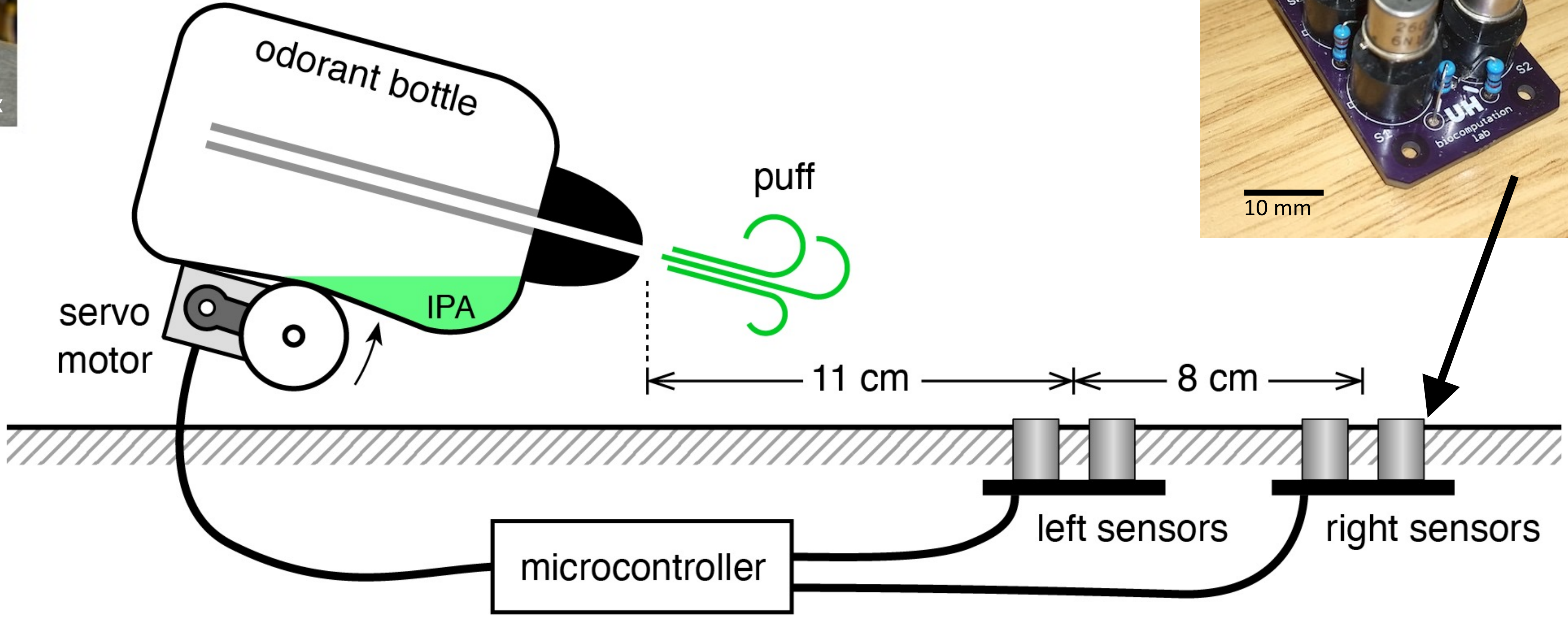
Speeding up MOx sensors with signal processing

- 24-bit ADCs at 180Hz increase resolution of amplitude and temporal dynamics
- Denoising via a constant-acceleration Kalman filter.
- Modifications to the KF system equations counteract the slow impulse response recovery



Drix & Schmuker, ACS Sensors 2021.

Application: Direction sensing



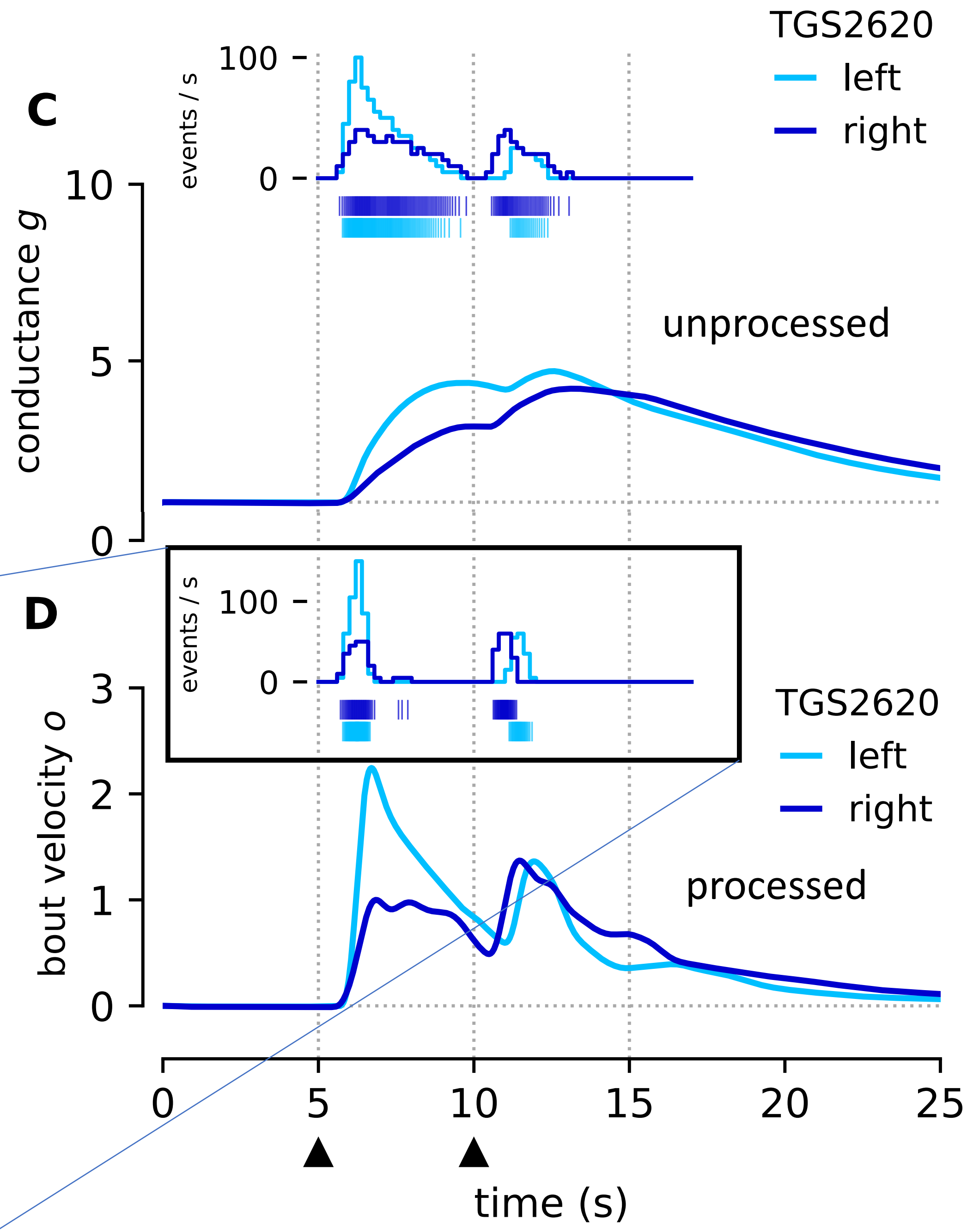
IPA = Iso-Propyl-Alcohol (not 🍺!!!)

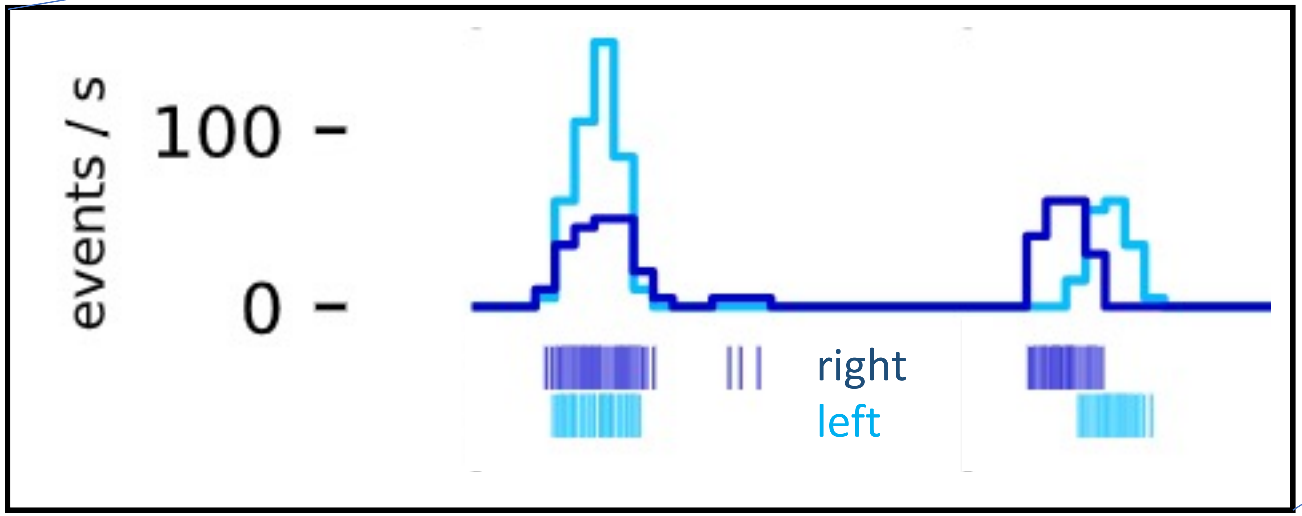
Drix & Schmuker, ACS Sensors 2021.

Fast event-based odor direction detection with slow MOx sensors

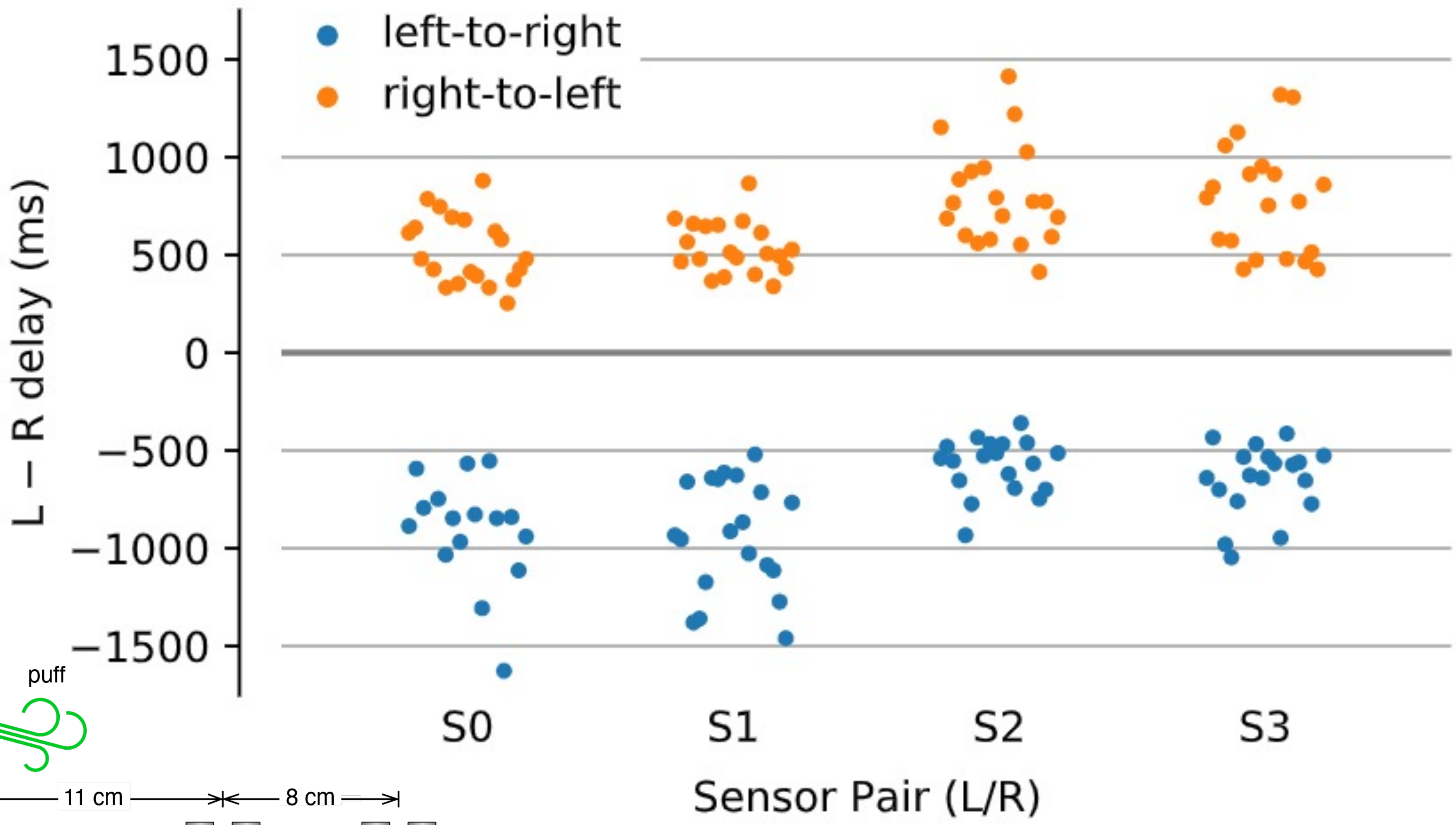
- Odor comes from the right.
- Signal processing accelerates sensor response.
- Event representation indicates faster onset.

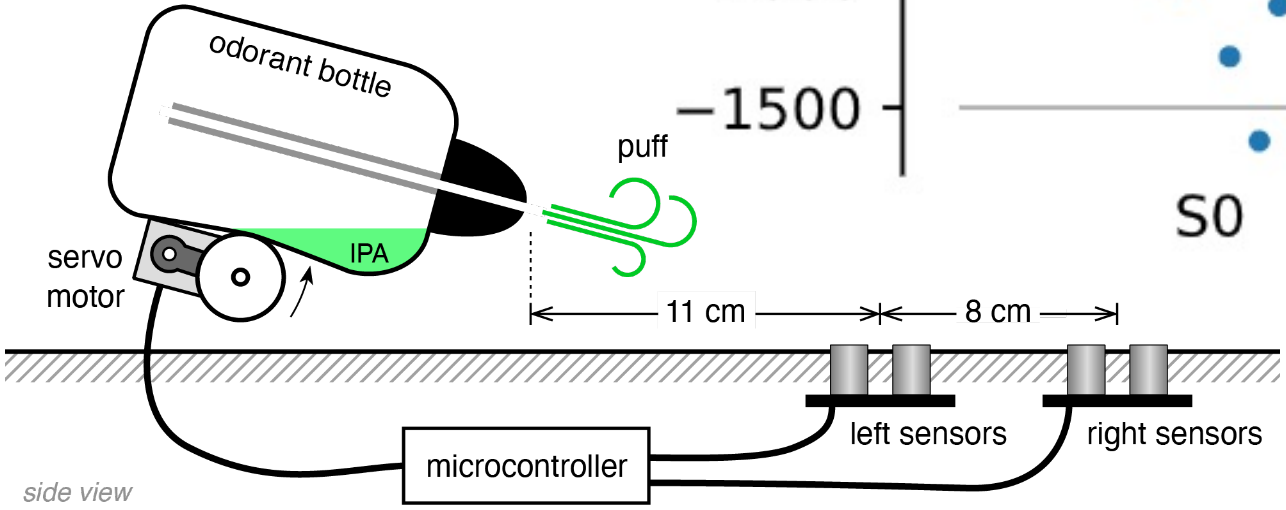
Drix & Schmuker, ACS Sensors 2021.





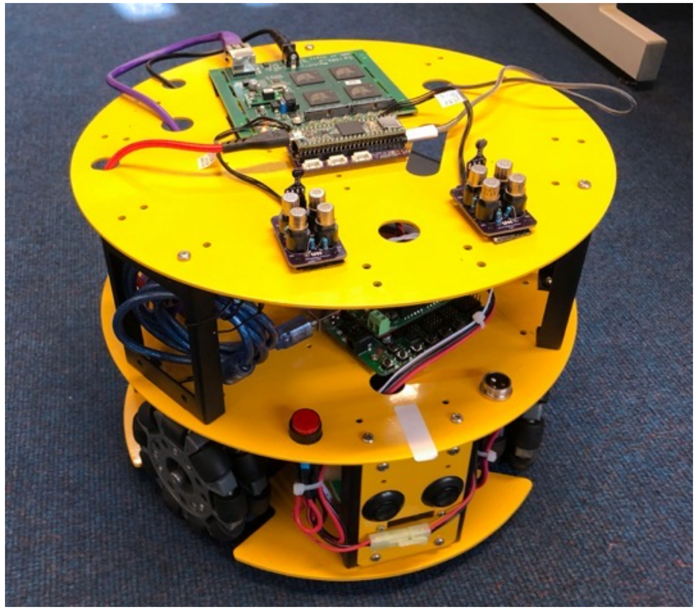
Sub-second resolution of time differences





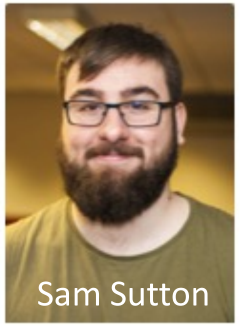
Drix & Schmuker, ACS Sensors 2021.

Navigation experiments (preliminary)

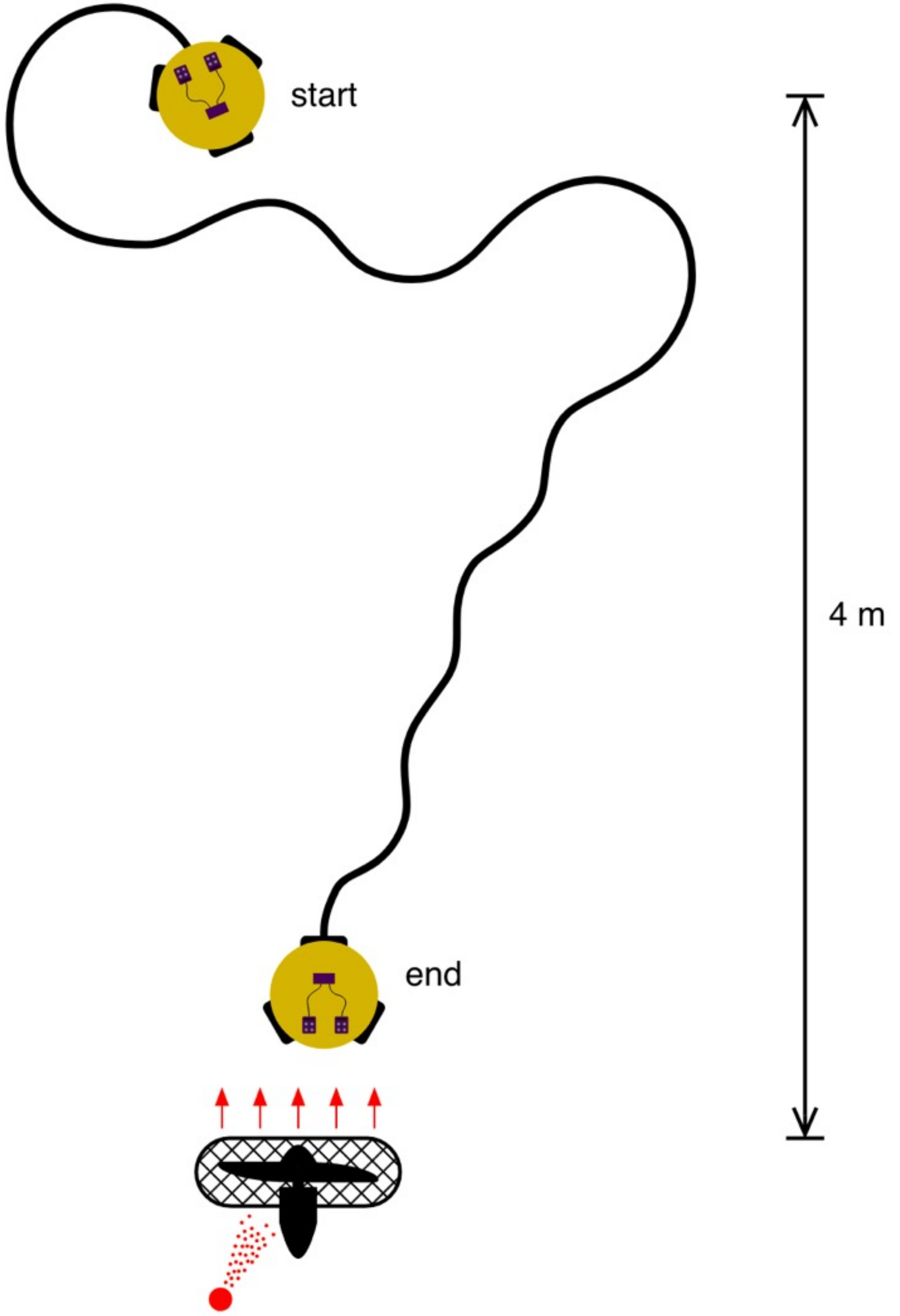


- Omnidirectional robot with stereo-osmic electronic nose.
- Event-based direction decoding on Neuromorphic hardware (That’s a separate talk ;)).
- Event-driven reactive odour search algorithm:
  - If odour is detected from left:
    - Turn left
    - Move forward
  - Vice versa for odour from right.
- Experiment: Robot must find a pulsed odour source.

Navigation experiments (preliminary)



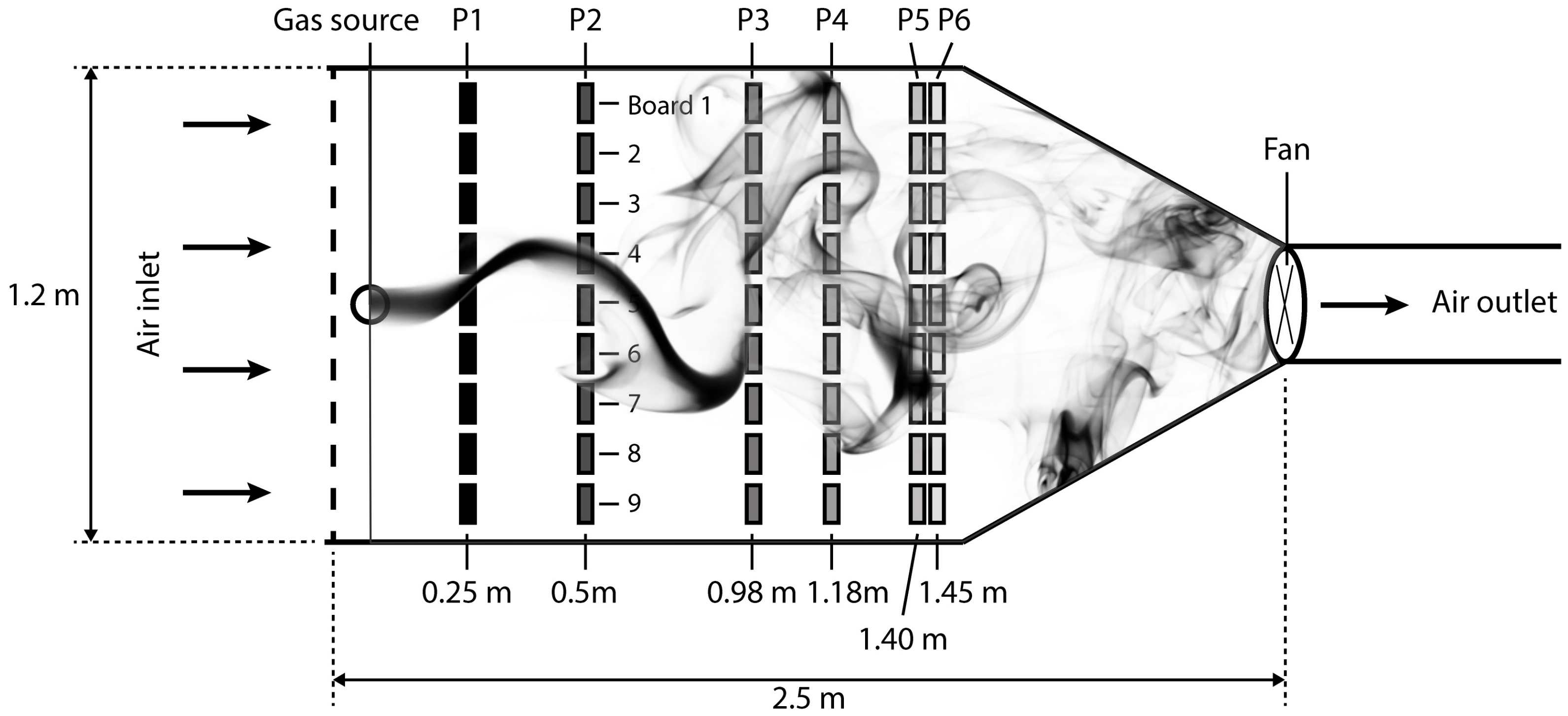
- Robot locates pulsed gas source.
- Reactive navigation creates casting & surging pattern
- One-off, last experiment before lockdown in March 2020 (more experiments planned)

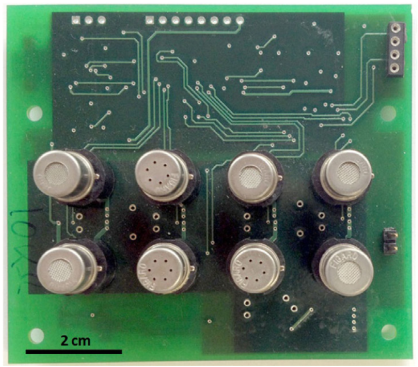


Observation: The robot trajectory resembles a typical "casting and surging" trace, as observed in insects.

Future work: use clues from bout statistics for navigation and assess goal finding performance.

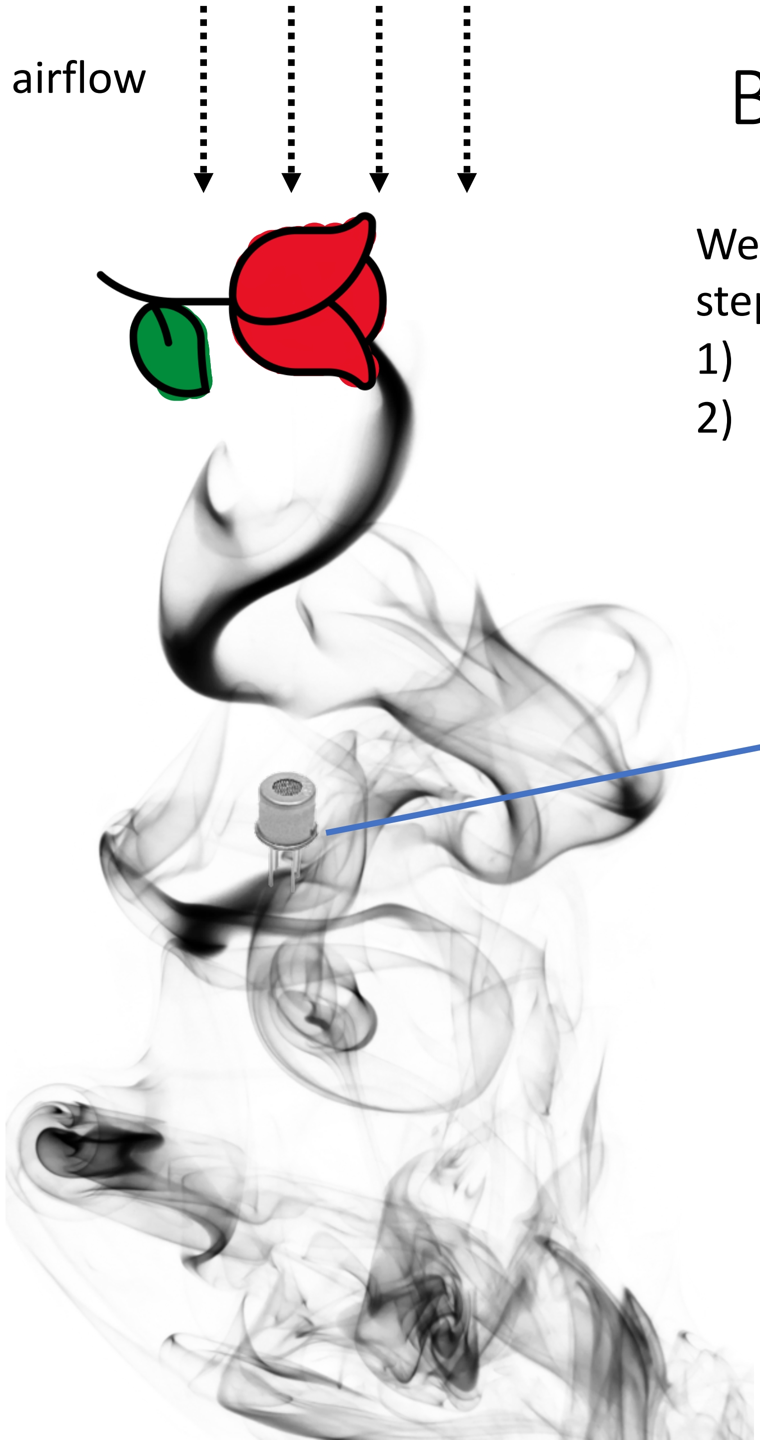
Gas sensor recordings in a wind tunnel





Gas sensor board

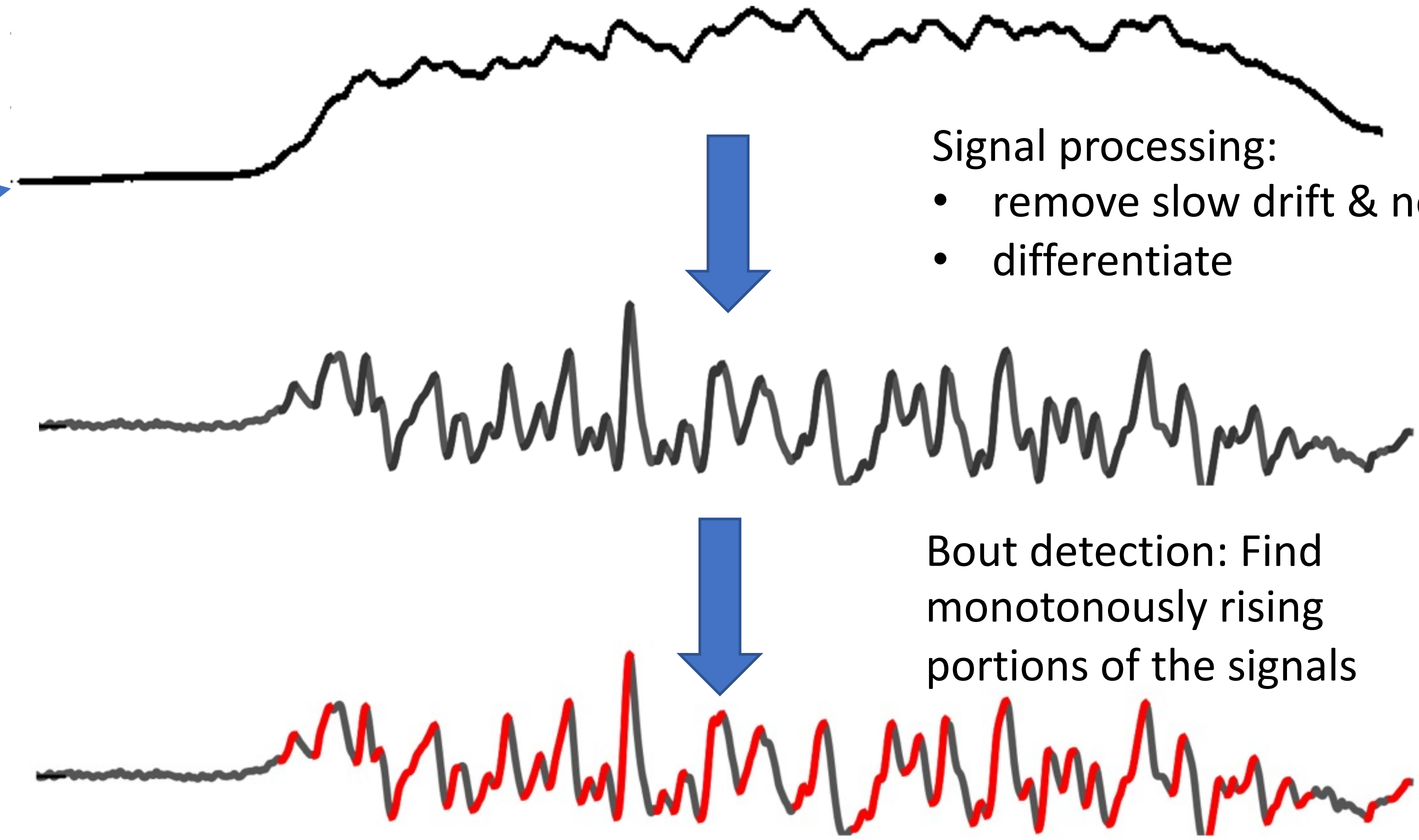
- Public wind tunnel data set (Vergara et al 2013).
- Sensors at varying down-wind and cross-wind distance from the odour source.



Bout statistics

We detect odor “bout” encounters in the gas sensor signal in three steps

1) Differentiate
2) Detect “Bouts”: monotonously rising portions of the signal

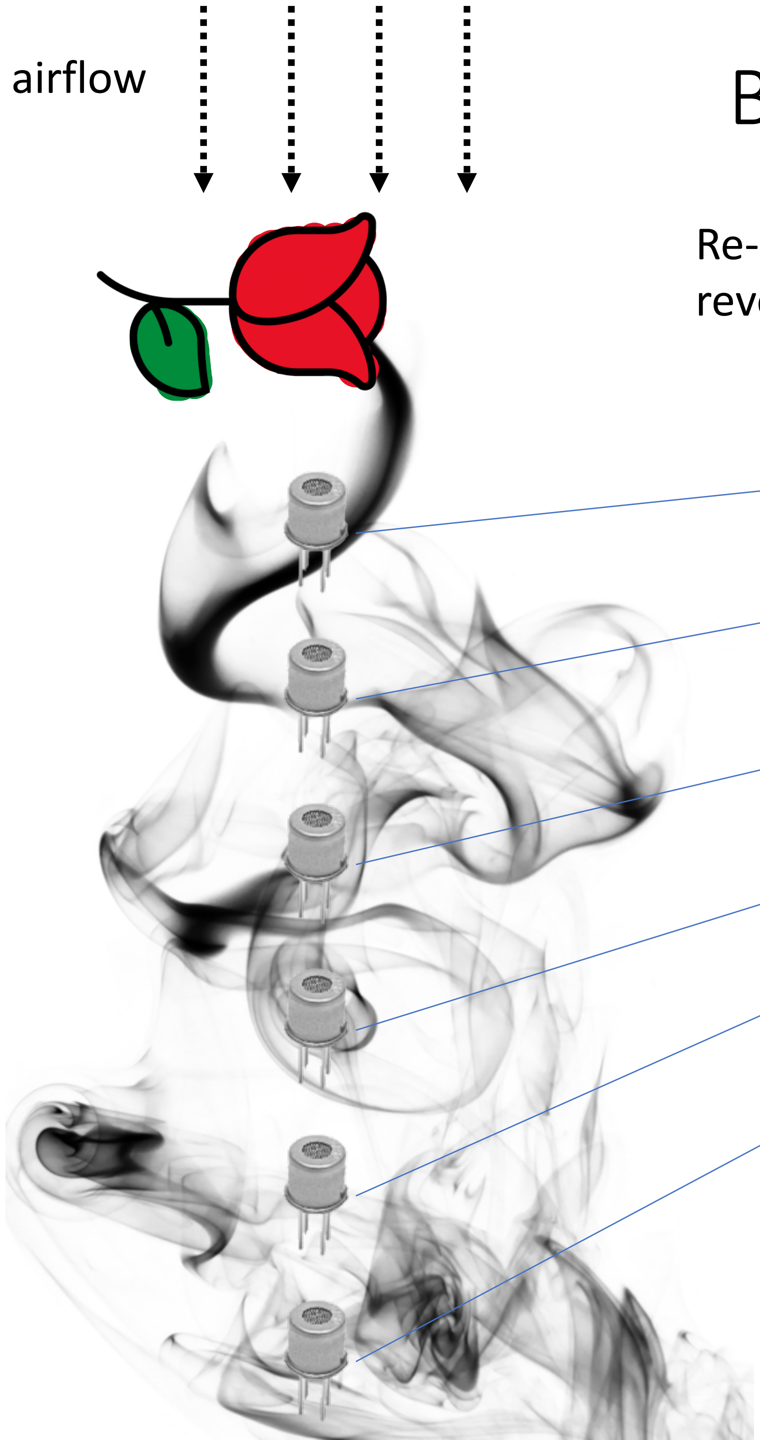


Signal processing:

- remove slow drift & noise
- differentiate

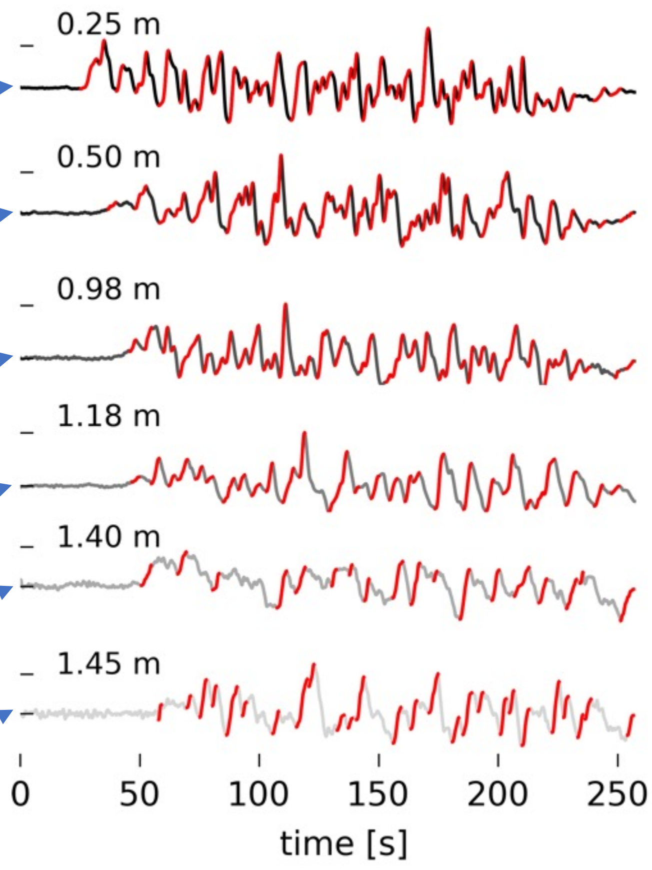
Bout detection: Find monotonously rising portions of the signals

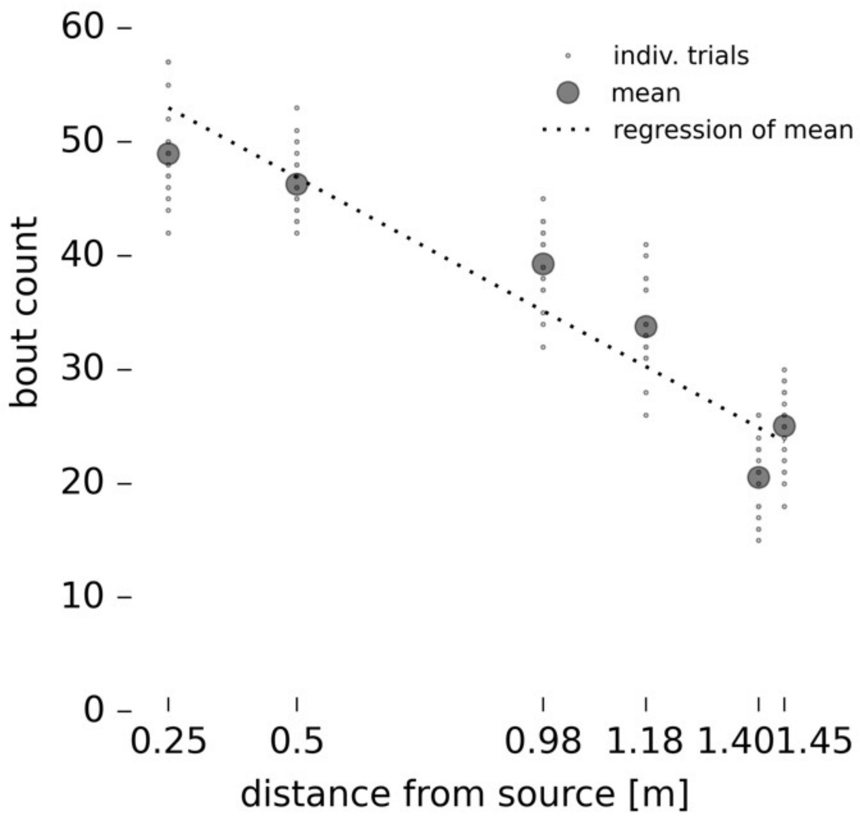
Schmuker et al., Sens Act Chem B, 2016.



Bout counts encode down-wind distance

Re-analysis of the Vergara dataset using "bout statistics"
revealed that the temporal structure of odorant plumes encodes source distance.

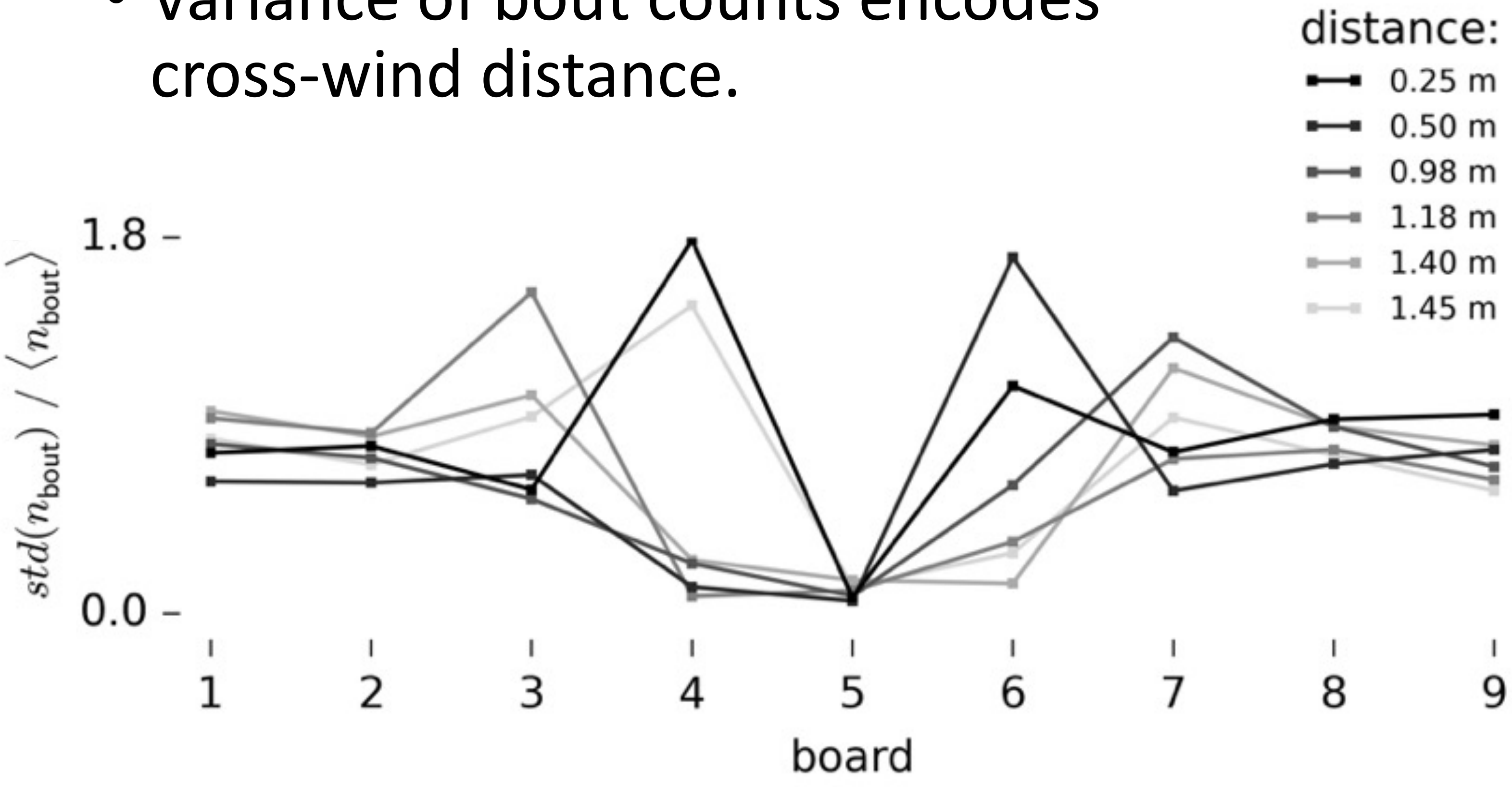


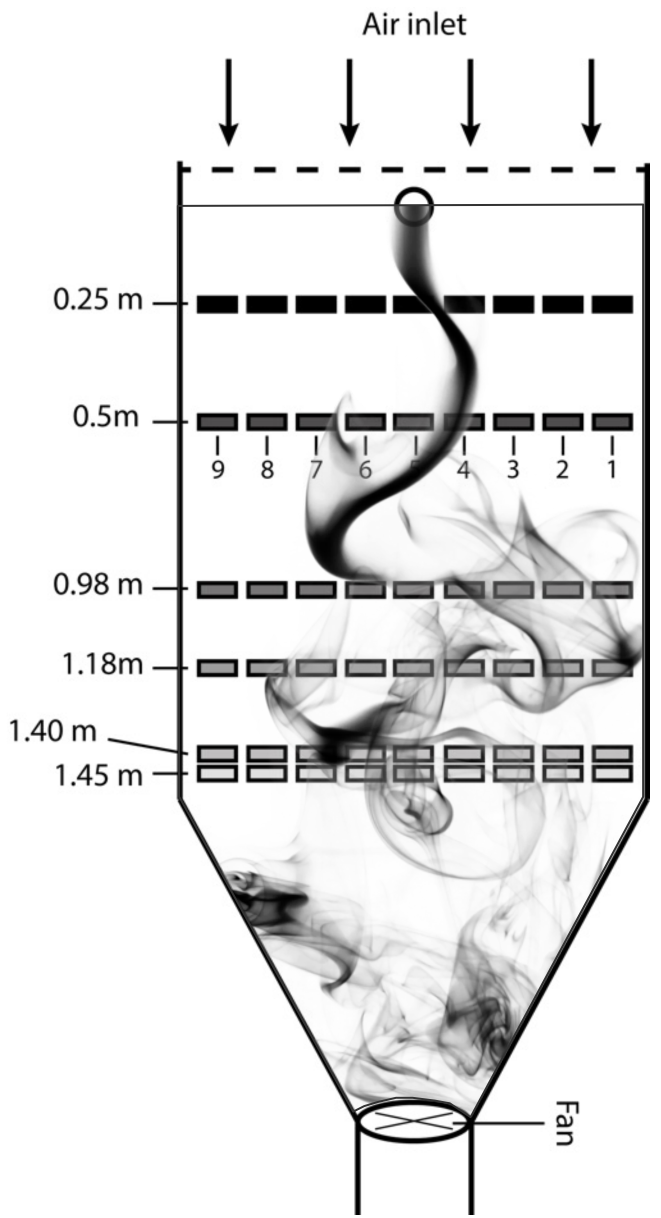


Schmuker et al., Sens Act Chem B, 2016.

Decoding Cross-wind distance

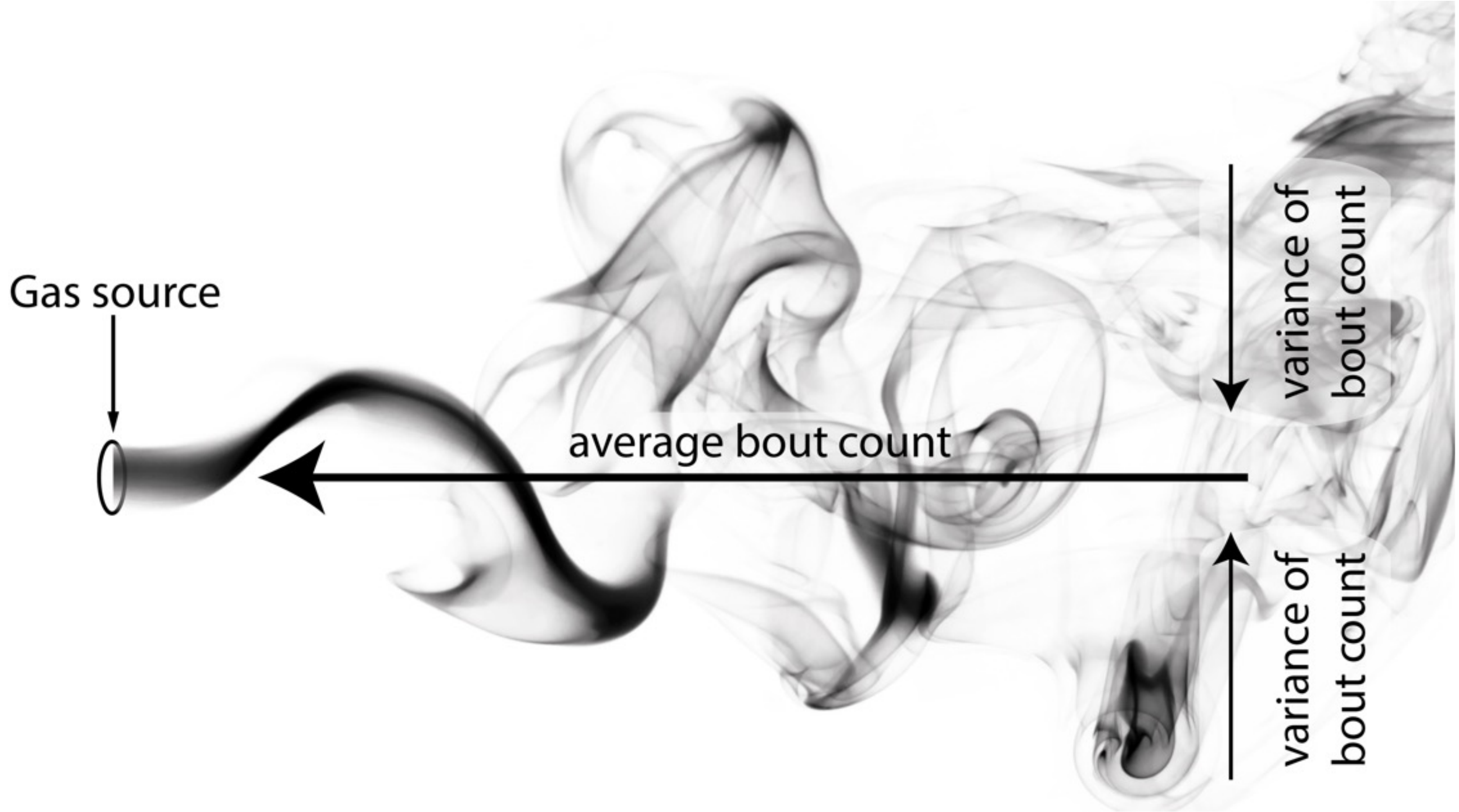
- Variance of bout counts encodes cross-wind distance.





Schmuker et al., Sens Act Chem B, 2016.

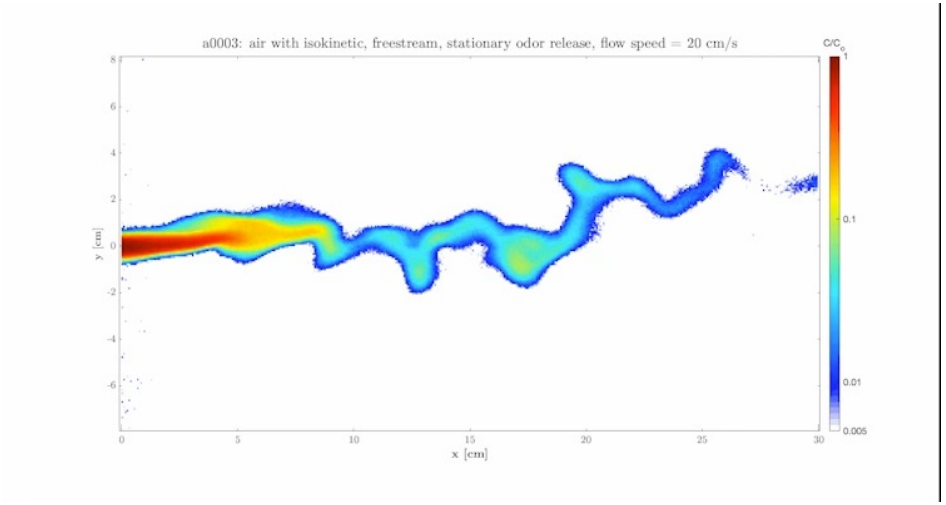
Clues for gas-based navigation



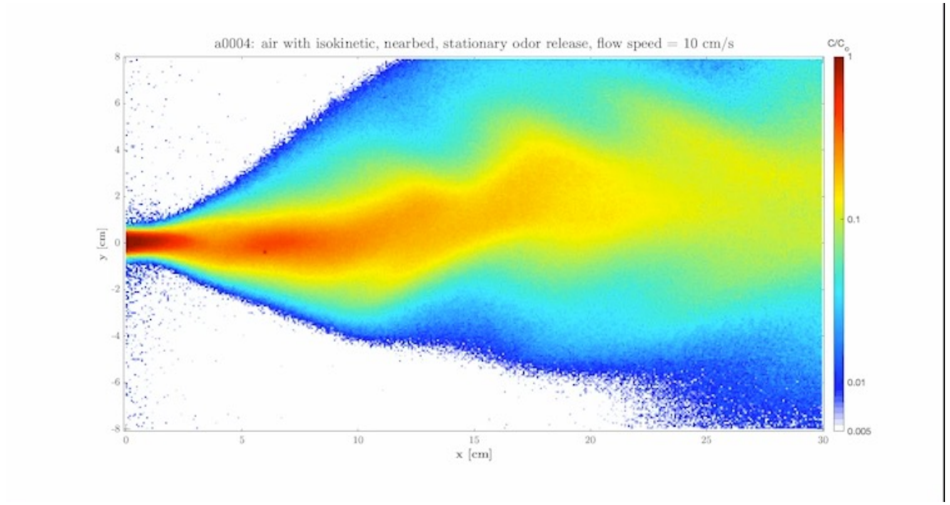
Schmuker et al., Sens Act Chem B, 2016.

Re-interpret: What's the timescale?

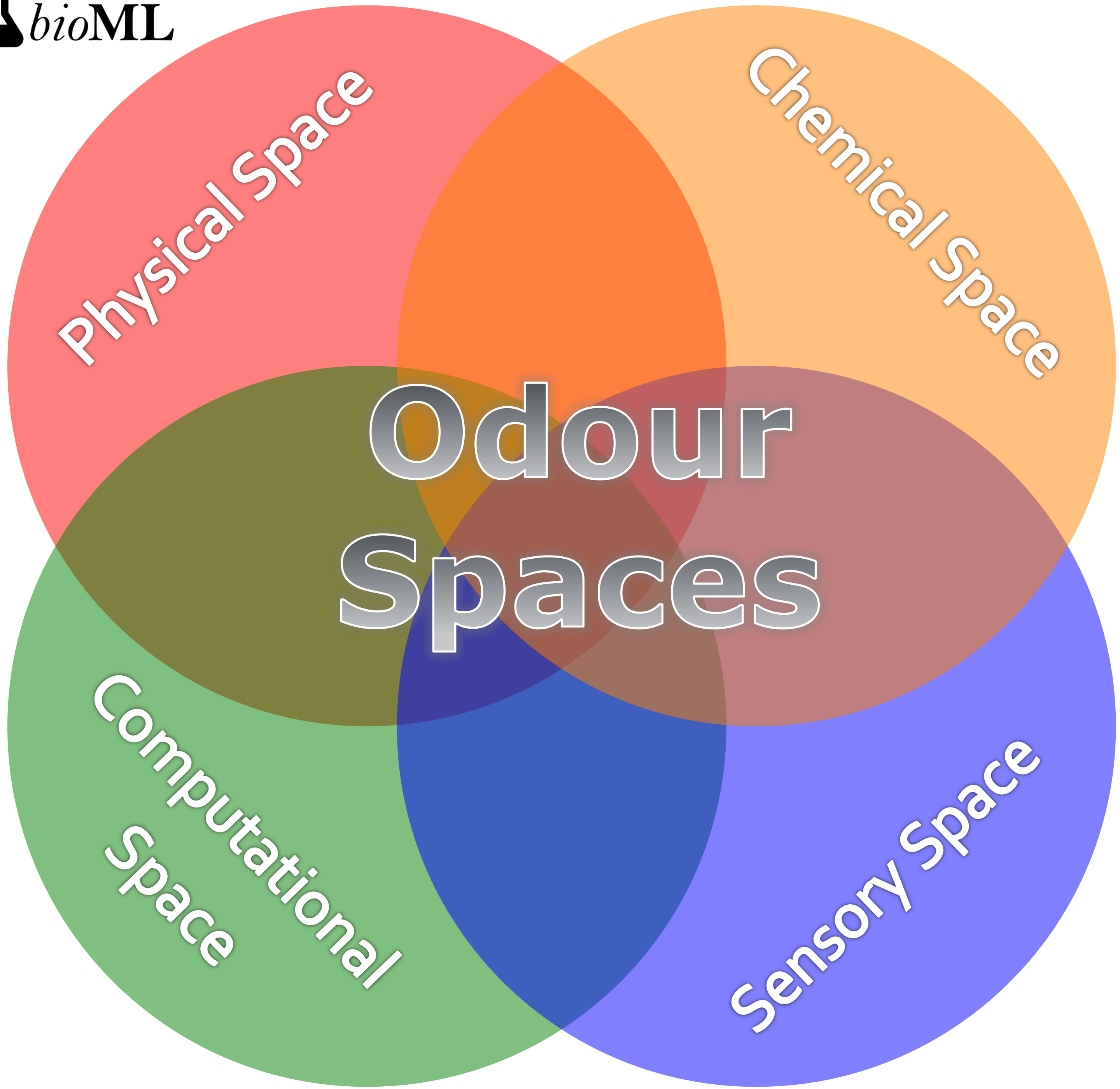
Free-flow



Near-bed



bioML

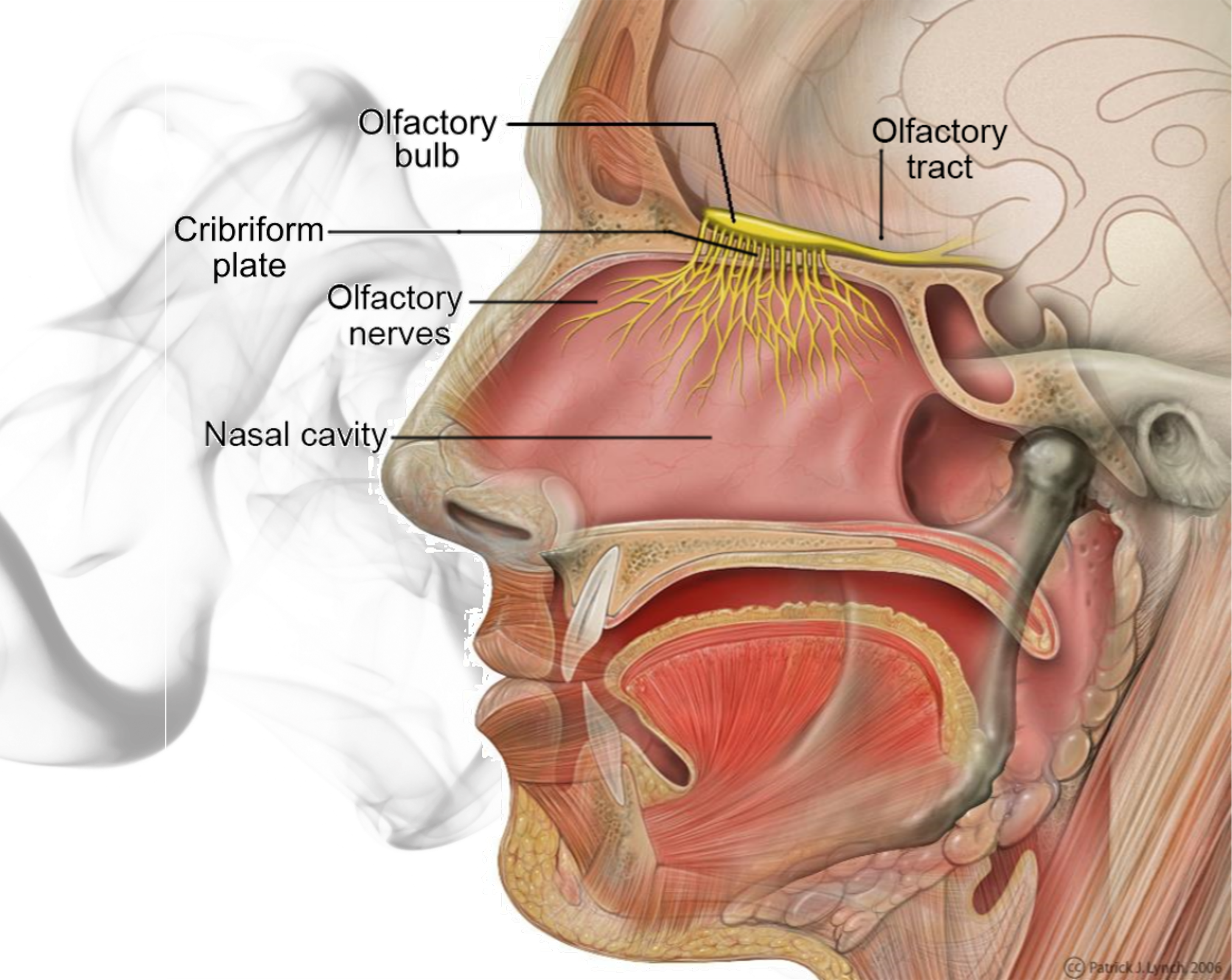


BioMachineLearning @

University of Hertfordshire UH

- Physical space: odour filaments in turbulent airflow.
- Chemical space: odorants.
- Sensory space: receptors and receptive fields.
- Computational space: neuronal networks.

Anatomy of olfaction

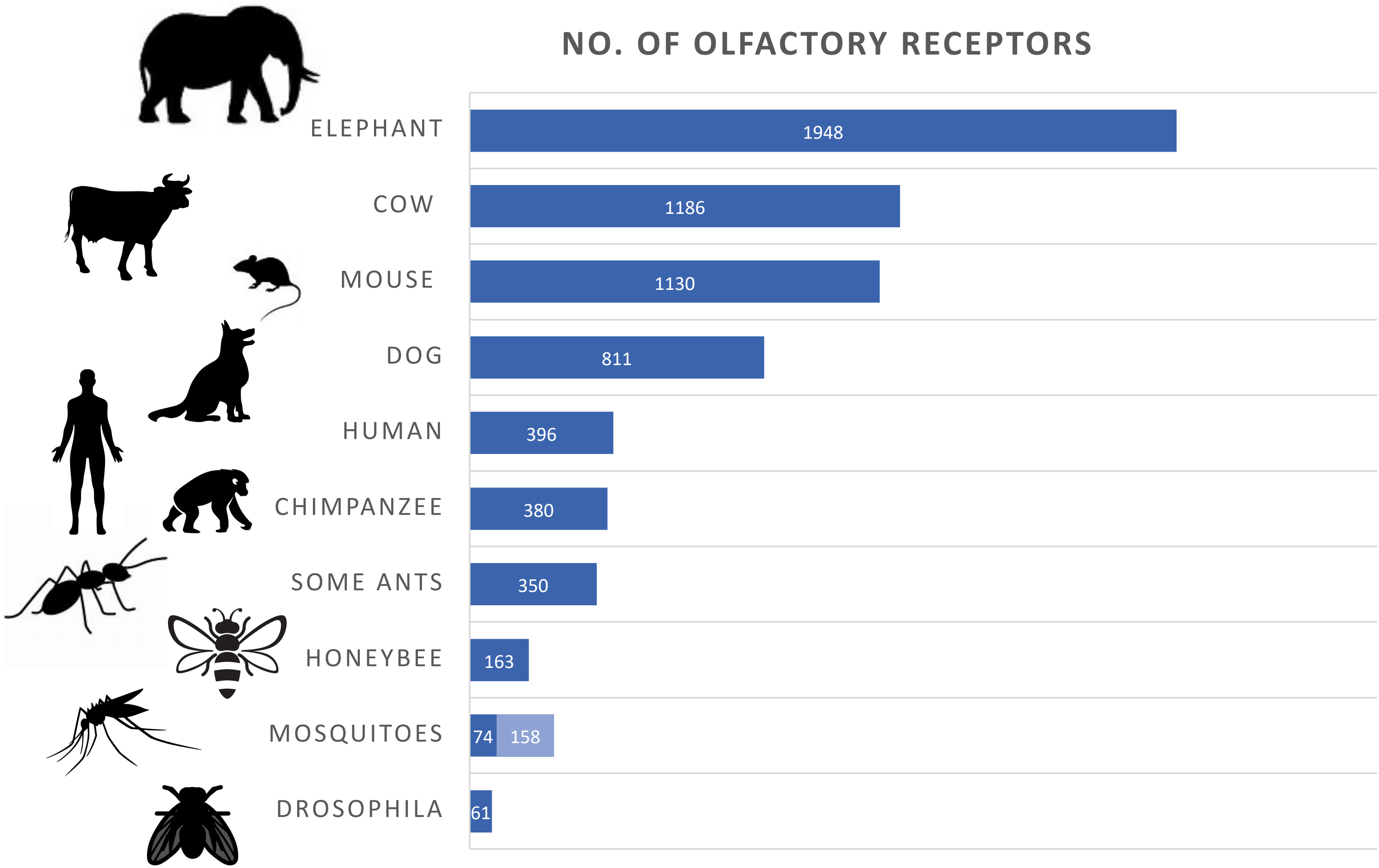


Number of odorant receptors across species

- Number of olfactory receptors varies widely across species
- Correlates roughly with olfactory ability

But open questions remain…

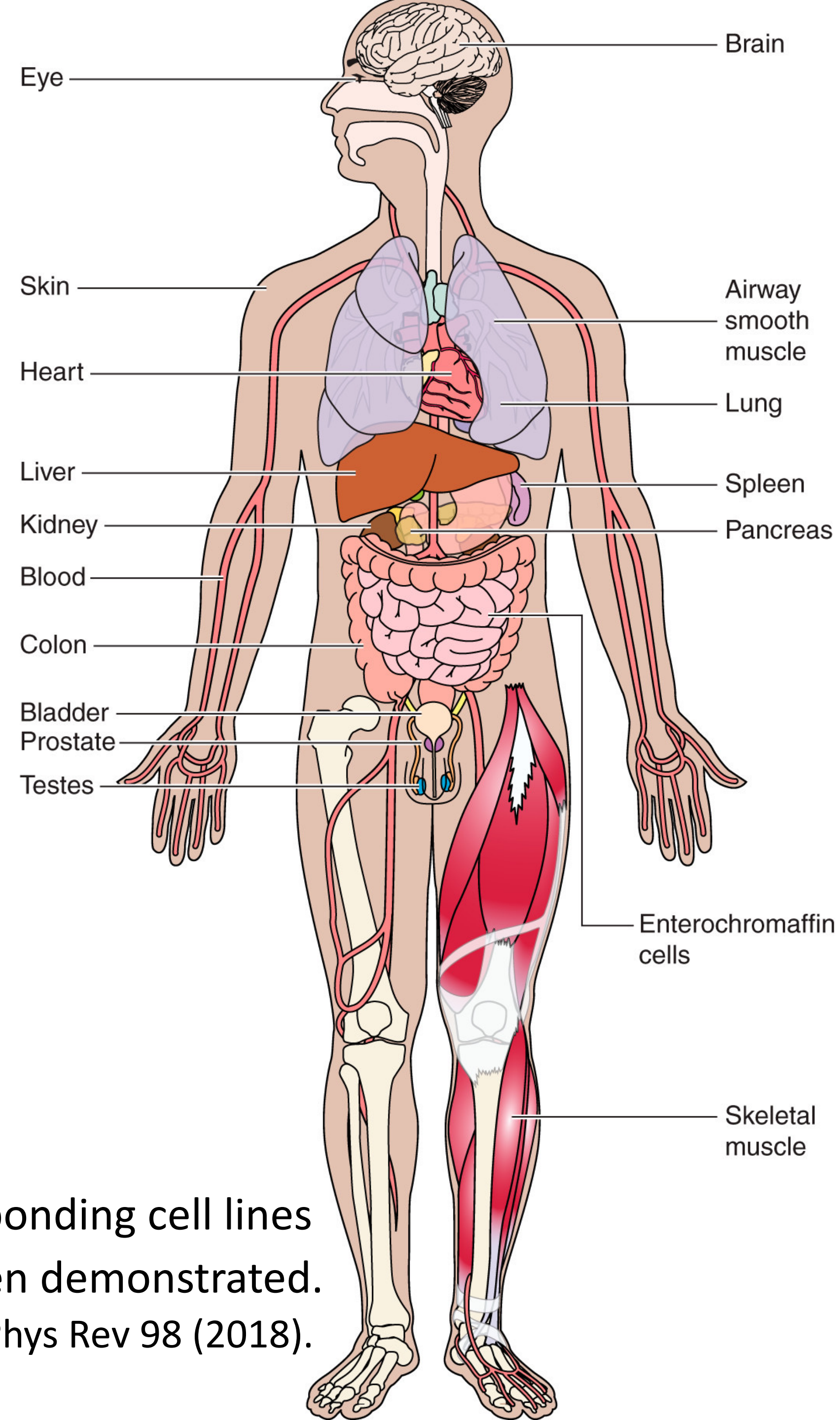
- High olfactory performance with low receptor count – Mosquitoes, honeybees
- *Cows?!?*



Adapted from Niimura et al., *Genome Res* (2014) with data from Zhou et al., PLoS Genetics (2012).

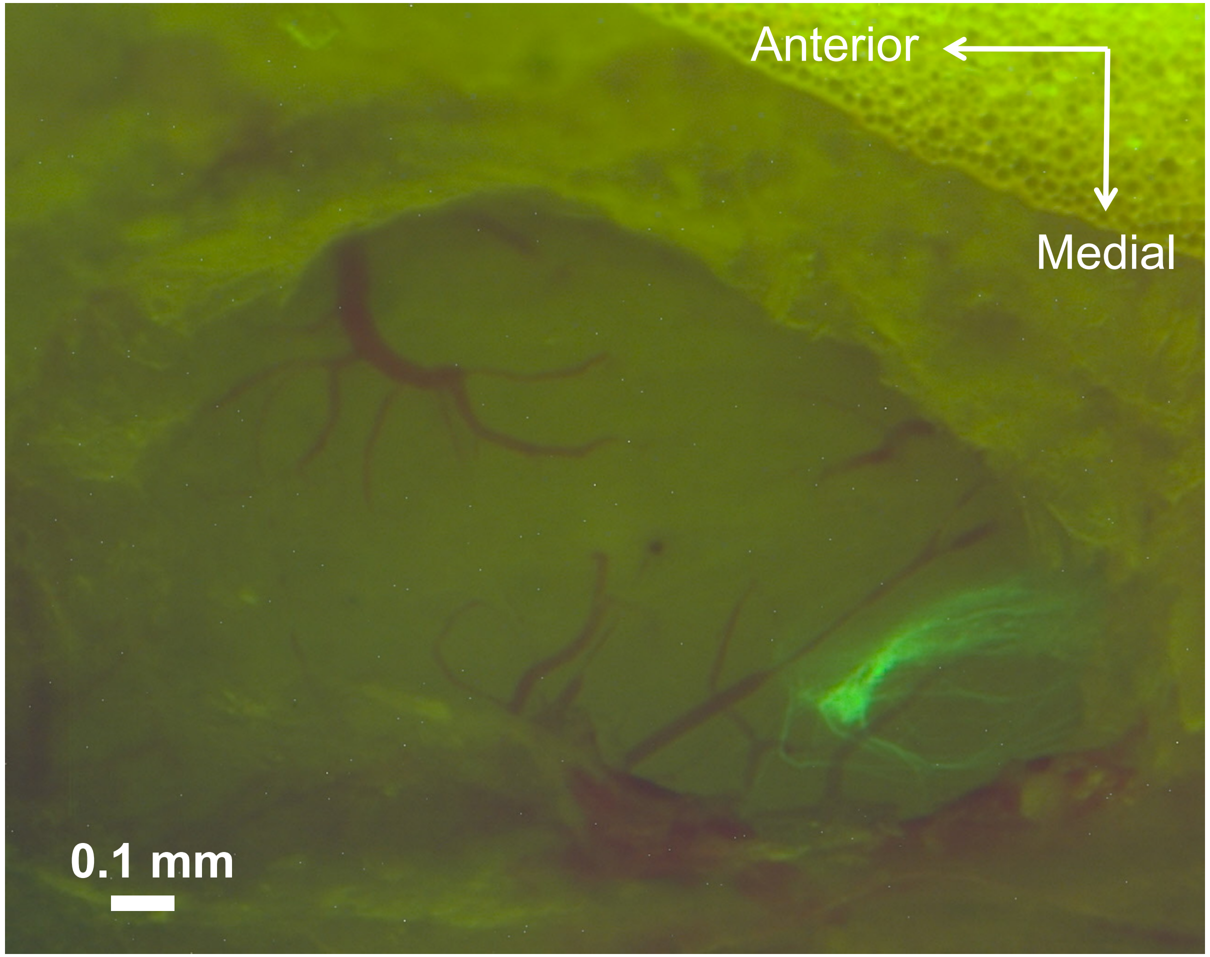
Odorant receptors are found in most tissues

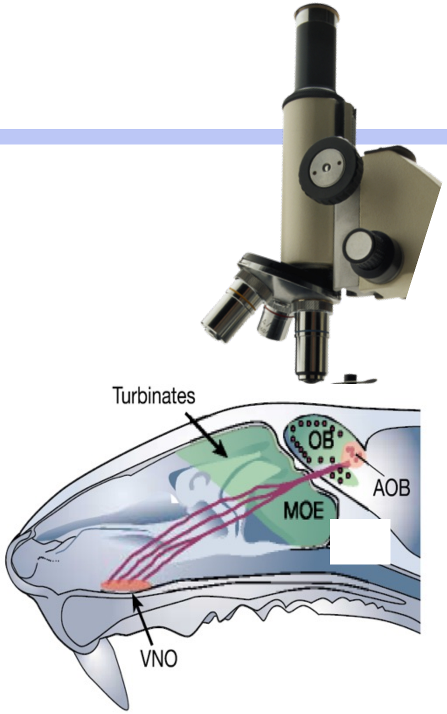
- Suggests functions beyond olfaction
- High expression levels in cancer cells highlight role as potential therapeutic targets.
- What do they sense?



Human tissues and corresponding cell lines in which OR functionality has been demonstrated.
From Maßberg & Hatt, Phys Rev 98 (2018).

Targeting a genetically labeled glomerulus

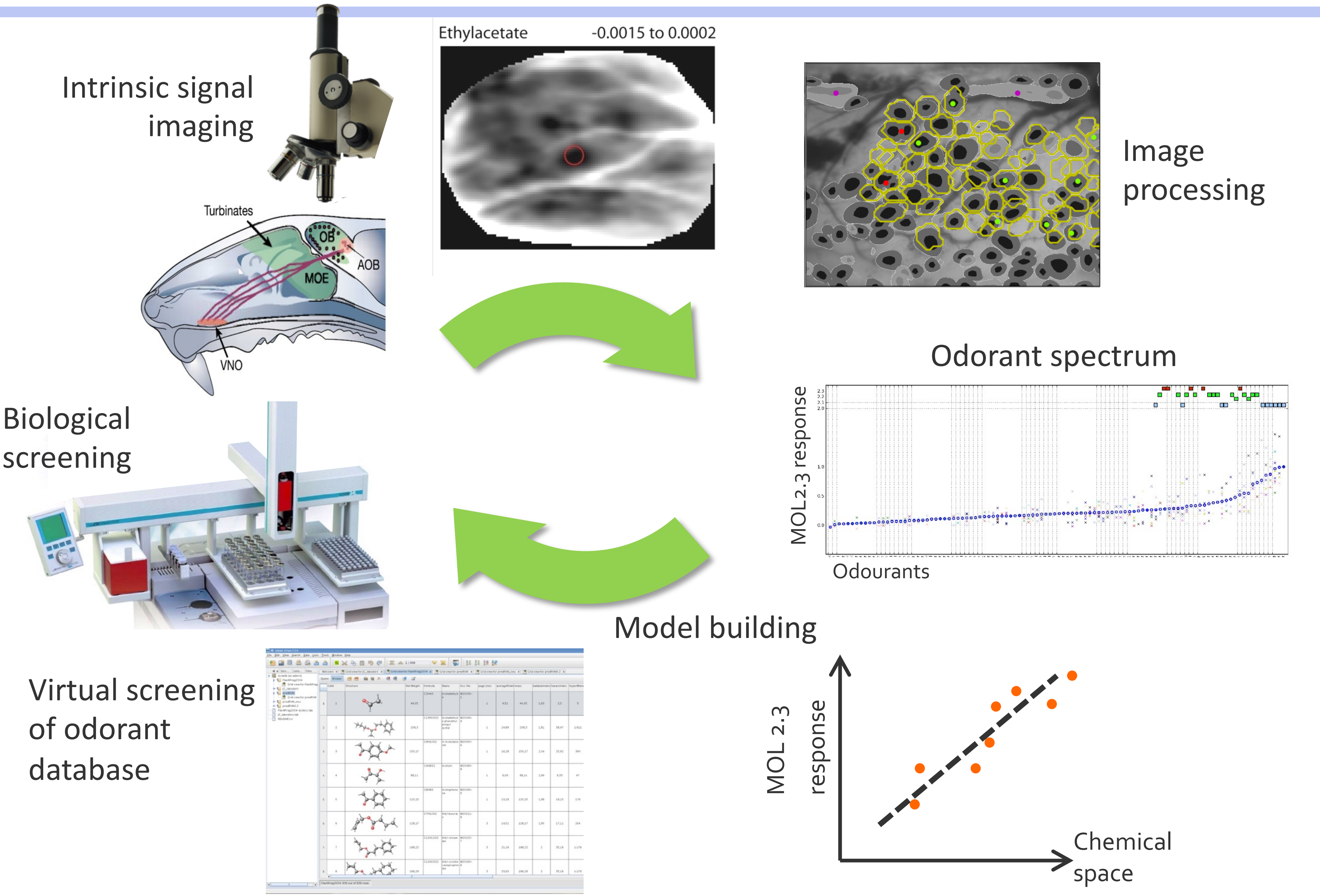




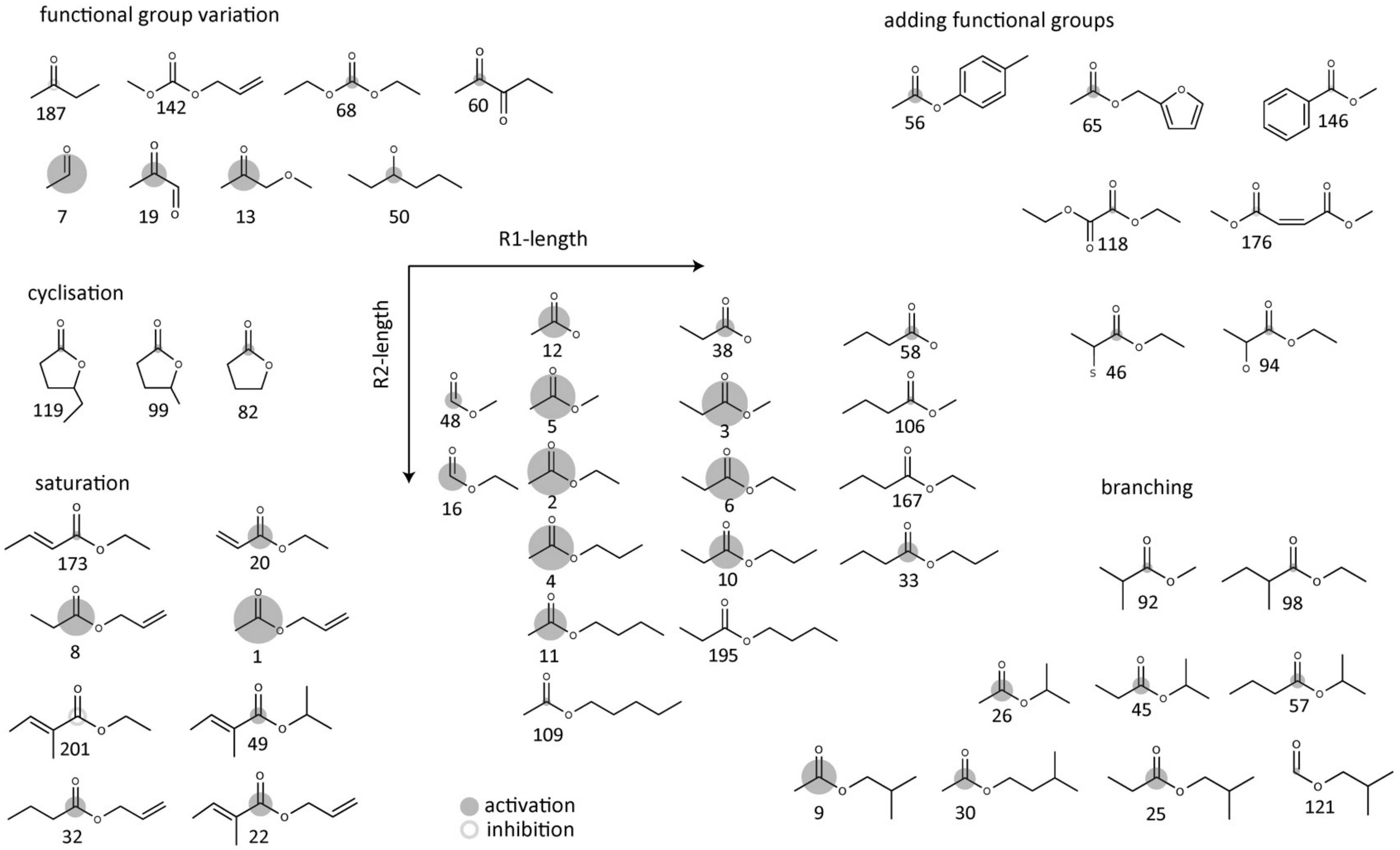
Hartwig Spors

Collaboration with Hartwig Spors
MPI for Biophysics, Frankfurt/Main, within DFG SPP1392

Iterative exploration of physiological space

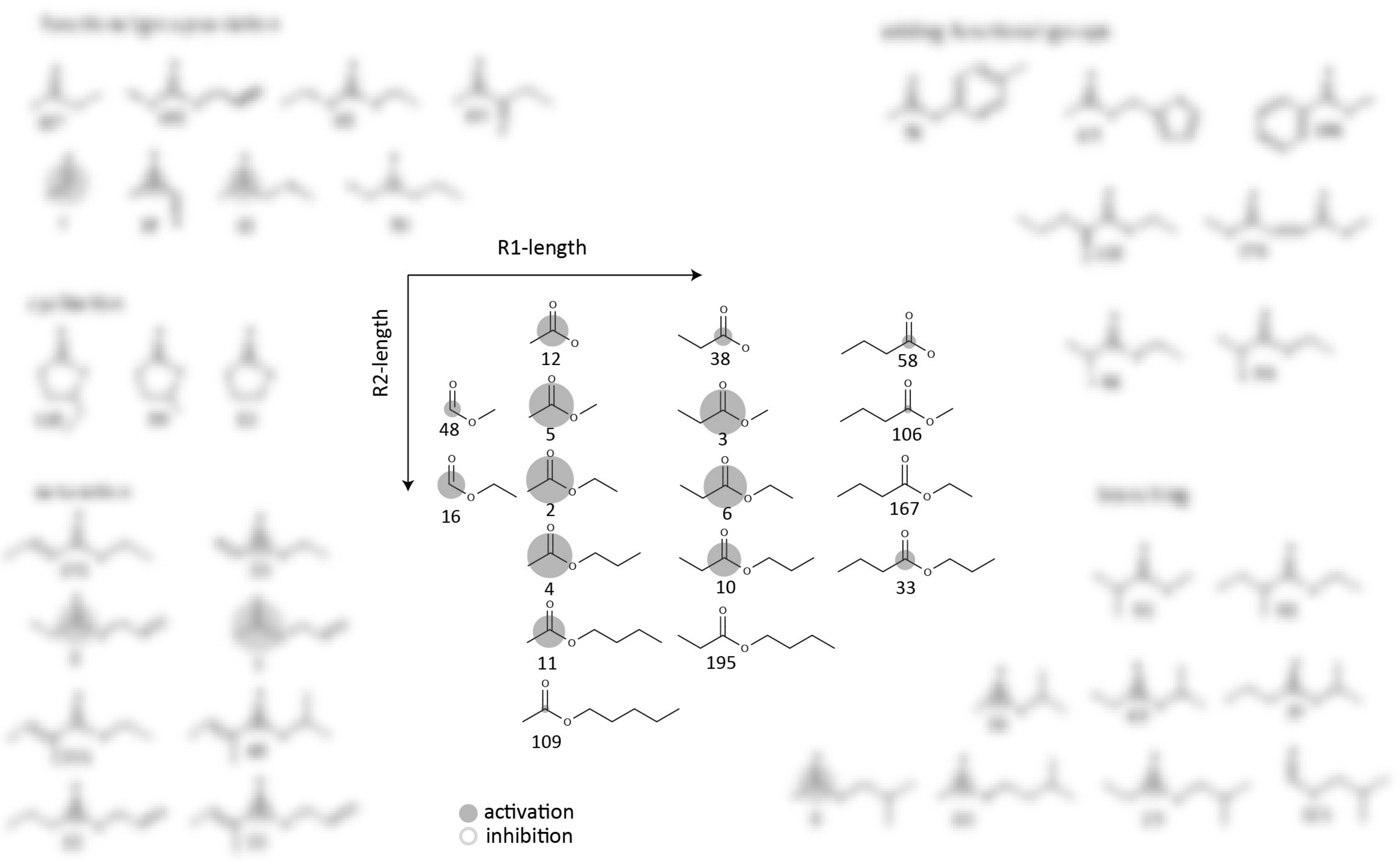


Ligand profile



"Fresh fruits, with exactly the right degree of ripeness, of the like that would go to KaDeWe, not Lidl or Aldi." – Christophe Laudamiel, Perfumer and Chemist.

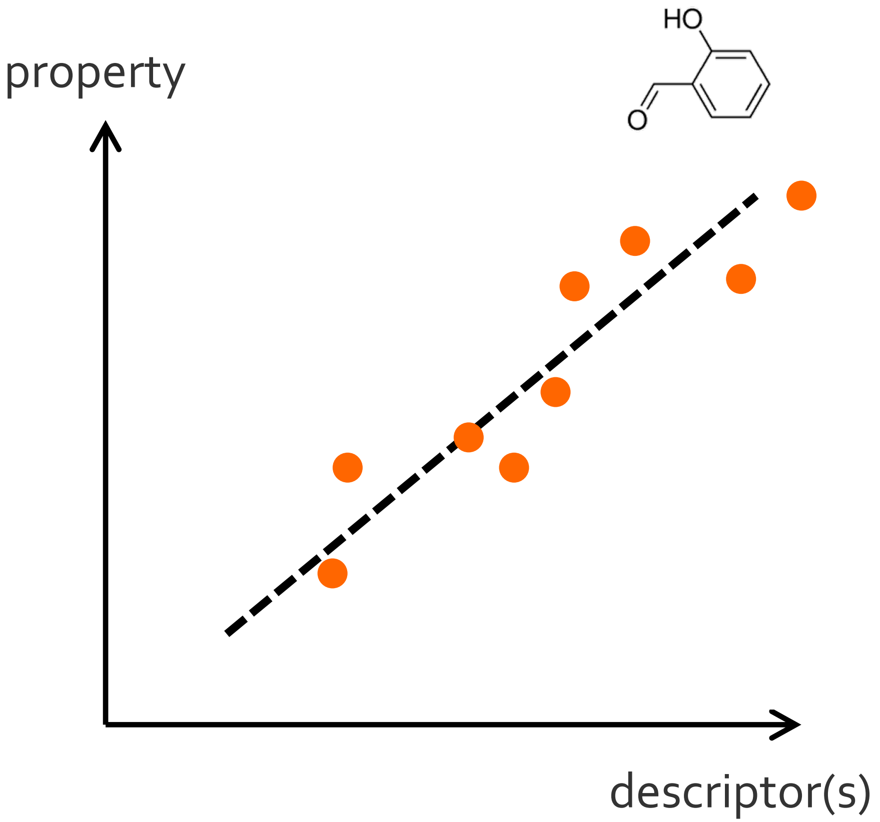
Ligand profile



"Fresh fruits, with exactly the right degree of ripeness, of the like that would go to KaDeWe, not Lidl or Aldi." – Christophe Laudamiel, Perfumer and Chemist.

Modelling molecular receptive fields with machine learning

- Encode molecules in a numerical representation of chemical space.
- In this space, multivariate statistics can be applied, e.g.:
  - Chemical similarity searching
  - Regression models
  - ML classifiers
- Goals:
  - Predict activity of odorants
  - Understand molecular receptive field

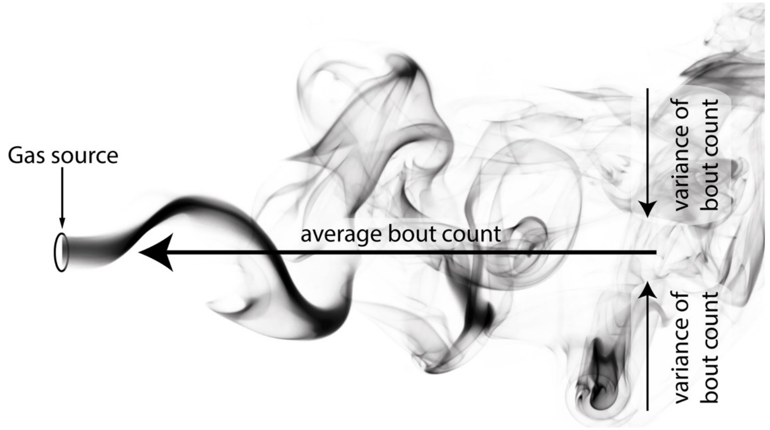


Gabler et al., *Molecular Informatics*, 2013.
Chen et al., *Chemical Senses*, 2011.
Eschbach et al., *Chemical Senses*, 2011.
Schmuker et al., *Chemistry Central Journal*, 2007.

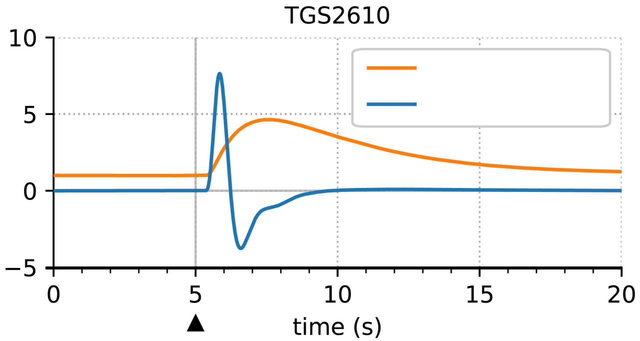
Which representation works best for odorants?

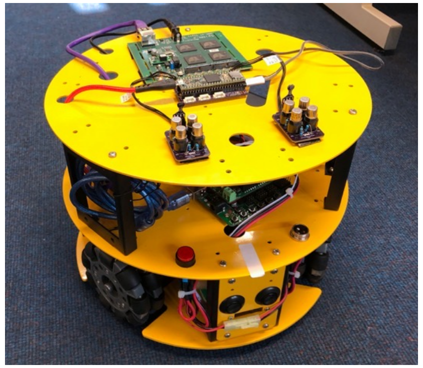
…. Ongoing research (not for sharing)

Summary



- Temporal dynamics of odorant plumes carry information about the olfactory scene.
- Gas sensors need high temporal resolution in order to be effective in natural, uncontrolled environments.
- Odour-based robot navigation benefits from fast sensors.
- Research into molecular representations for computational olfaction





Students, Postdocs and Funding

Students & Postdocs:

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Active Funding:

MRC Medical Research Council

NeuroNex ODOR2ACTION

European Union H2020

NEUROTECH
H2020 FETPROACT CSA
community building around
neuromorphic technology

Human Brain Project

THE ROYAL SOCIETY

Former Funding:

DFG
SPP 1392: Integrative Analysis of Olfaction

Olfaction SPP

Bundesministerium für Bildung und Forschung

bccn

Marie Curie IEF

European Regional Development Fund

AgRIA

VolkswagenStiftung