Feature extraction from sensor dynamics in an Electronic Nose

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1. Electronic what ?!

Definition

An electronic nose (eNose) is a device which is composed of **chemical sensors** and a **pattern-recognition system** for recognising odours [1].

Machine Learning stage

It produces a signature when an odour is introduced. ML algorithms are then used to identify the odour.

However, our eNose outputs up to **∼100 time series**, from which we need to **extract a smaller set of relevant features**.
The solution proposed here is to extract them from a **physical model**.

Applications

Biomedical engineering, Food-processing industry, Mine-clearing, Cosmetics, Olfactive navigation...

2. NeOse

Our work is based on the NeOse eNose, developed by Aryballe Technologies, a French start-up located at CEA in Grenoble:

Fig. 1: NeOse device.

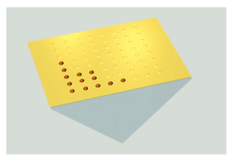


Fig. 2: Chemical sensors are peptides (small proteins) which are dropped off on the golden surface of a prism.

Imaging technique :
A light beam is sent to and reflected by the surface. When interactions occur, the refraction index changes and thus the reflected light too (fig. 3).

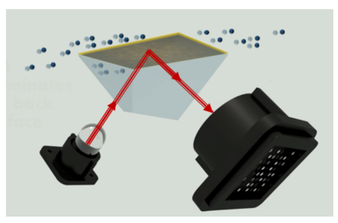


Fig. 3: Imaging technique principle.

3. Data acquisition

① Baseline acquisition
② Gas on at $t = t_s$
③ Gas off at $t = t_e$

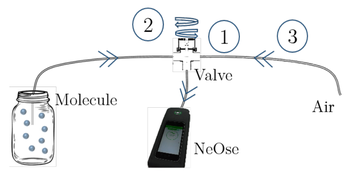


Fig. 4: Acquisition plan.

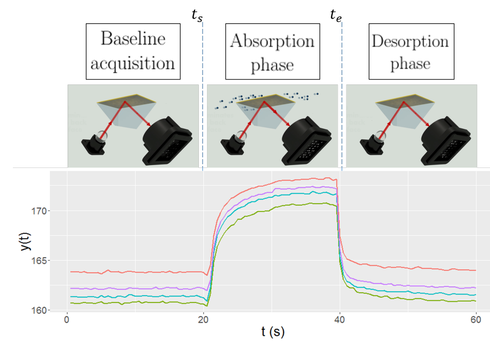
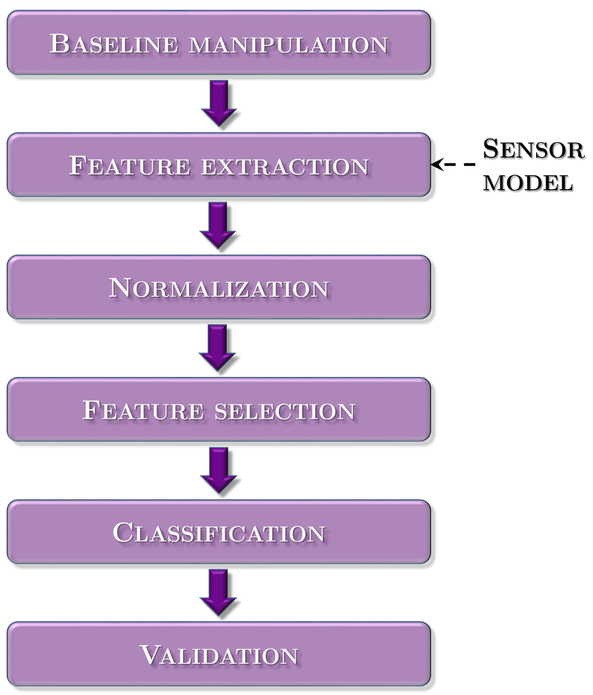


Fig. 5: Each line corresponds to the temporal response $y(t)$ of one peptide during an experiment as described above.

4. Data processing

Data are usually processed according to the plan [2]:



5. Sensor model

Molecular interaction

For each peptide $\mathcal{P}$, the following **binding reaction** occurs when a molecule $\mathcal{M}$ is introduced:

$$\mathcal{M} + \mathcal{P} \underset{\text{rate of desorption } k_d}{\overset{\text{rate of absorption } k_a}{\rightleftharpoons}} \mathcal{MP}$$

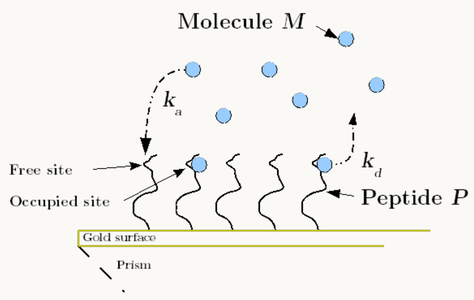


Fig. 7: Simplified molecular interaction.

Langmuir model

From this 1st order reaction, the kinetic of complex formed $\mathcal{MP}$ is obtained using the **kinetics parameters** k_a and k_d:

$$\underbrace{\frac{\mathrm{d}[\mathcal{MP}](t)}{\mathrm{d}t}}_{\substack{\text{change in \# of}\\ \text{occupied sites}}} = \underbrace{k_a[\mathcal{M}](t)[\mathcal{P}]}_{\substack{\text{Number of sites}\\ \text{becoming occupied}}} - \underbrace{k_d[\mathcal{MP}](t)}_{\substack{\text{Number of occupied}\\ \text{sites becoming free}}}$$

$$\iff \frac{\mathrm{d}\theta(t)}{\mathrm{d}t} = k_a[\mathcal{M}](t) - k_d\theta(t) \quad , \theta(t) = \frac{[\mathcal{MP}](t)}{[\mathcal{P}]}$$

Under some assumptions, Langmuir model arises [3]:

$$\theta(t, k_a, k_d) = \begin{cases} 0 & \text{if } t \leq t_s \\ \frac{k_a}{k_a+k_d}(1 - e^{-(k_a+k_d)(t-t_s)}) = \theta_a(t) & \text{if } t \in [t_s, t_e[\\ \theta_a(t_e)e^{-k_d(t-t_e)} & \text{if } t \geq t_e \end{cases}$$

The imaging technique doesn't measure directly the fraction of occupied site θ but a linear transformation of it:

$$y(t, \alpha, k_a, k_d) = \alpha\theta(t, k_a, k_d)$$

where α depends on molecule $\mathcal{M}$ mass, peptide $\mathcal{P}$ concentration and temperature → thus, **not on the interaction**!

6. Results

Model fitting

The Langmuir model is fitted using nonlinear least-squares (with BFGS).

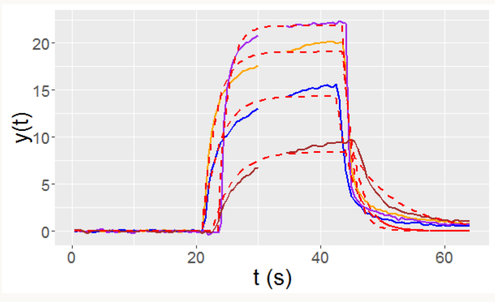
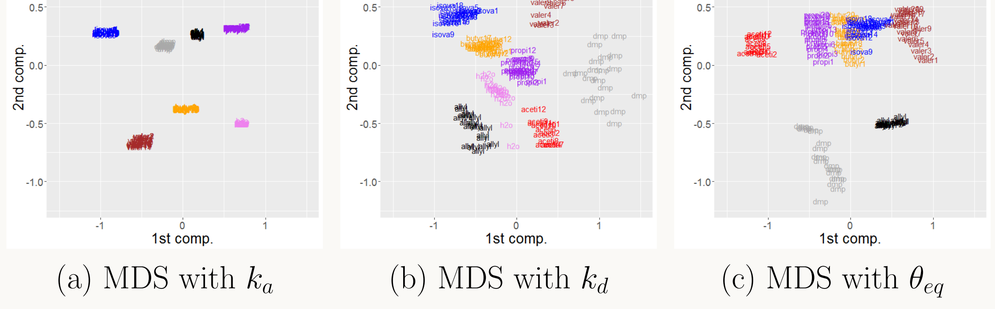


Fig. 8: Solid lines are real data after baseline subtraction (**butyric-acid**, **isovaleric-acid**, **propionic-acid**, **valeric-acid**) and dashed lines the fitted values.

Multi-Dimensionnal Scaling and Classification

Data set : 8 molecules, repeated 20 times at constant temperature.



(a) MDS with k_a (b) MDS with k_d (c) MDS with θ_{eq}

Fig. 9: MDS results (**acetic-acid $C_2H_2O_2$**, **propionic-acid $C_3H_6O_2$**, **butyric-acid $C_4H_8O_2$**, **valeric-acid $C_5H_{10}O_2$**, **isovaleric-acid $C_5H_{10}O_2$**, **dimethylpropane**, **allyl-hexanoate**, **water**).

We use the features (k_a, k_d and θ_{eq}, the static response) in a classifier such as **k-NN** and **SVM**. Each feature gives **a cross-validated score of 100%**.

7. Discussion

Conclusion

- Langmuir model explains well the absorption but is sometimes poor in the desorption phase.
- The features extracted from the dynamics are reproducible and discriminative.

Perspectives

- Explain desorption patterns.
- Collect larger and harder data set.

Acknowledgments

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[1] J. W. Gardner and P. N. Bartlett, "A brief history of electronic noses," Sensors and Actuators B: Chemical, vol. 18, no. 1, pp. 210–211, Mar. 1994.
[2] R. Gutierrez-Osuna, "Pattern analysis for machine olfaction: a review," IEEE Sensors journal, vol. 2, no. 3, pp. 189–202, 2002.
[3] Y. Hou et al., "Continuous Evolution Profiles for Electronic-Tongue-Based Analysis," Angew. Chem. Int. Ed., vol. 51, no. 41, pp. 10394–10398, Oct. 2012.

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