1. Electronic what ?!

**Definition**
An electronic nose (eNose) is a device which is composed of chemical sensors and a pattern-recognition system for recognizing 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 Arysta LifeScience, a French start-up located at CEA in Grenoble.

**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 changes (Fig. 3).

**Molecular interaction**
For each peptide, the following binding reaction occurs when a molecule M is introduced:

\[ M + P \rightarrow \text{complex} \]

From this 1st order reaction, the kinetic of complex formed is obtained using the kinetics parameters \( k_1 \) and \( k_2 \):

\[
\frac{d[M][P]}{dt} = k_1[M](t) - k_2[M][P](t)
\]

**Sensor model**

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\[
\frac{d[M][P]}{dt} = k_1[M](t) - k_2[M][P](t)
\]

**Langmuir model**

The Langmuir model explains well the absorption but is sometimes poor in the desorption phase.

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

3. Data acquisition

**Fig. 4:** Acquisition plan.

- Baseline acquisition
- Gas on at \( t = t_s \)
- Gas off at \( t = t_0 \)

4. Data processing

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

- Feature selection
- Feature extraction
- Normalization
- Classification
- Validation

5. Sensor model

**Fig. 7:** Simplified molecular interaction.

**Multi-Dimensional Scaling and Classification**

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

**Fig. 9:** MDS with \( k_1 \) and \( k_2 \)

(a) MDS with \( k_1 \)
(b) MDS with \( k_2 \)
(c) MDS with \( \theta \)

We use the features \( (k_1, k_2, \theta) \), the static response in a classifier such as k-NN and SVM. Each feature gives a cross-validated score of 100%.

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.

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**
- Collect larger and harder data set.

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