Blind Source Separation under the Langmuir model for chemical sensors

IEEE SAM

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July 10, 2018

Electronic what ?

An electronic nose = bio-inspired instrument which is able to identify and recognise Volatile Organic Compounds (VOCs) [1]

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How does it work ?

Electronic nose
Principle

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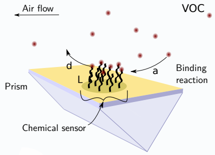

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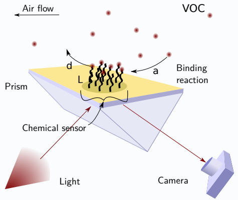

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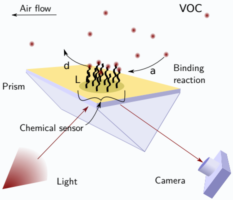

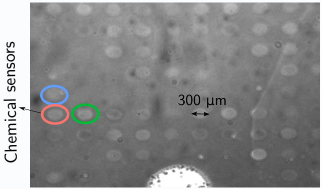

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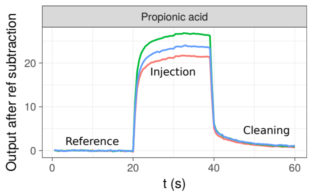

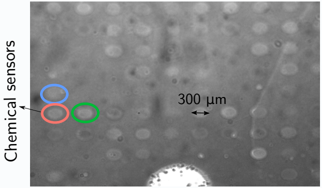

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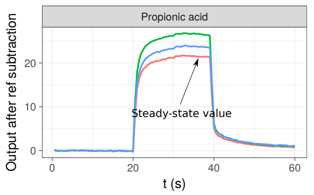

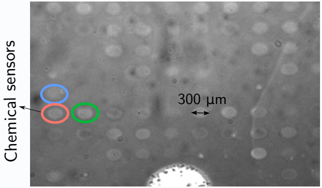

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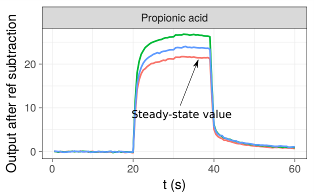
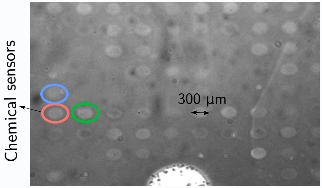
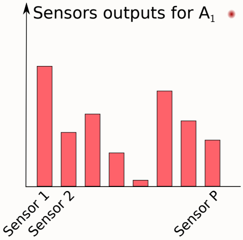


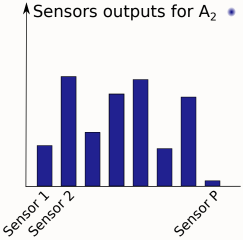


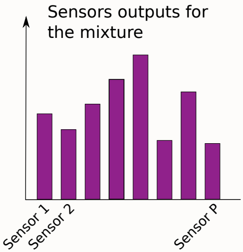
For what purpose ?

Biomedical, in/outdoor air monitoring, security, navigation, ...

Electronic nose
Source Separation issue







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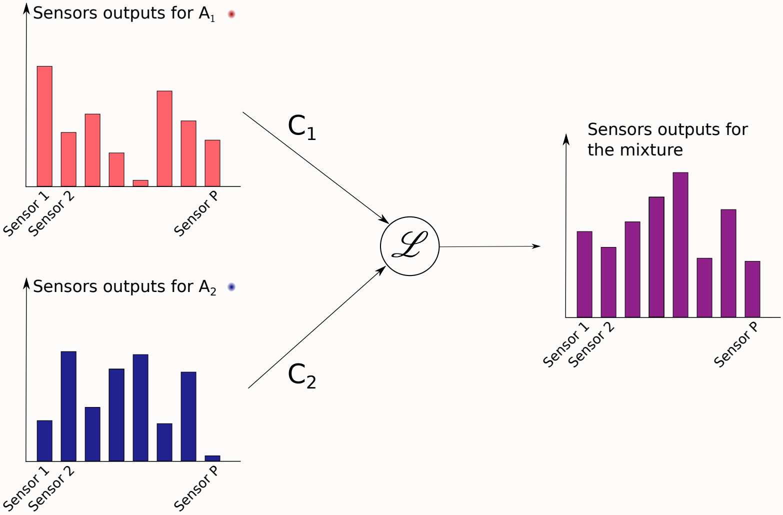

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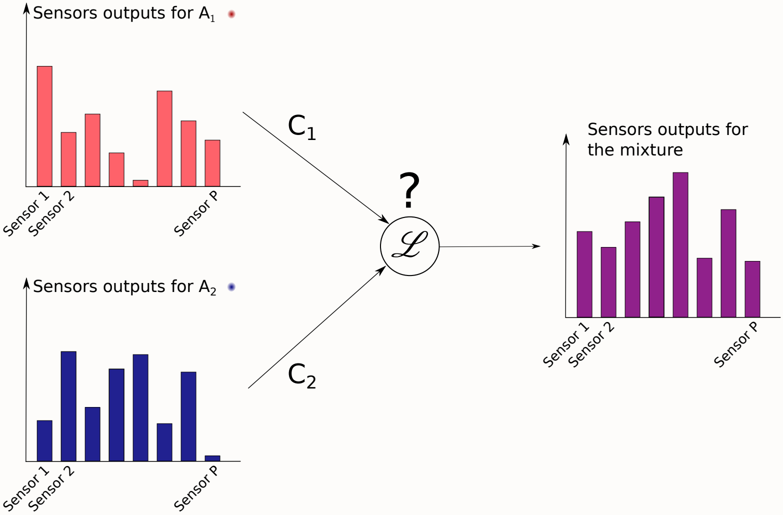

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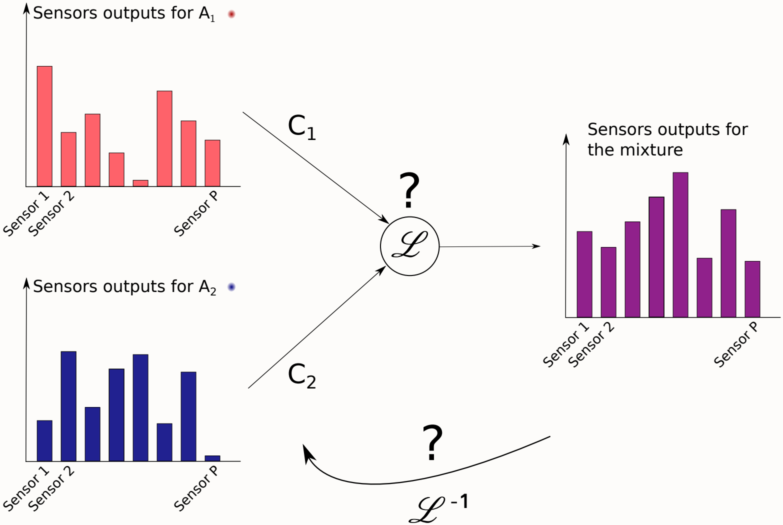

Langmuir isotherm

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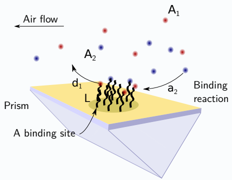

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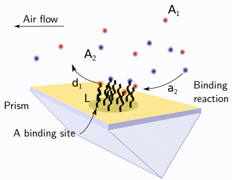
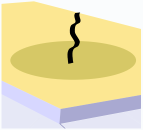
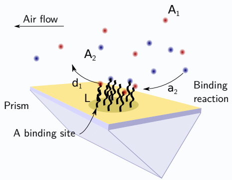
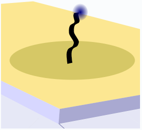




Free site

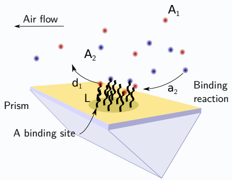
Langmuir isotherm

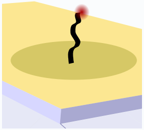




Occupied site

Langmuir isotherm

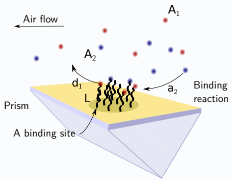


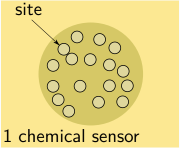


Occupied site

Physico-chemical mixture model
Chemical model

Langmuir isotherm





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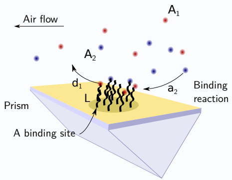

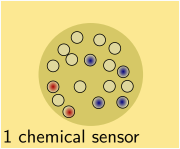

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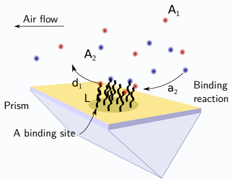
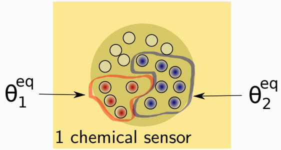
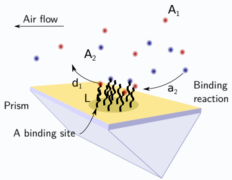
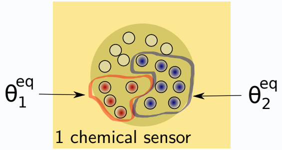




θ^{eq} : fraction of occupied sites

Langmuir isotherm





θ^{eq} : fraction of occupied sites

Langmuir isotherm [2] for a multi-component gas, noting :

- r the VOC
- p the chemical sensor
- n the mixture

$$\theta^{eq}_{rpn} = \frac{k_{rp} c_{rn}}{1 + \sum_{r=1}^{R} k_{rp} c_{rn}}$$

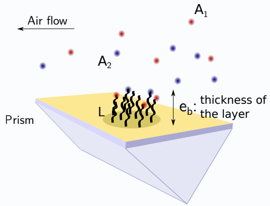
with k_{rp} the **affinity** and c_{rn} the **concentration**

Surface Plasmon Resonance model

Additivity assumption

Physico-chemical mixture model
Optical model

Surface Plasmon Resonance model



Assuming that e_b **is in the nanometer range**, the measure y_{rpn} is **proportional** to the fraction of occupied sites θ_{rpn}^{eq} (with m_r the mass of $\mathcal{A}_r$) [3, 4]:

$$y_{rpn} = \gamma m_r \theta_{rpn}^{eq}$$

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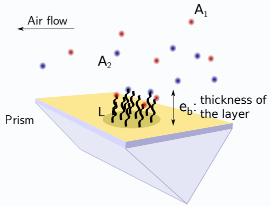

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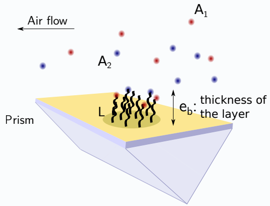

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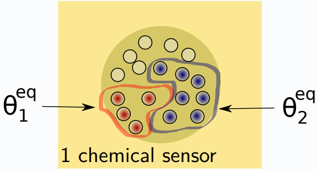

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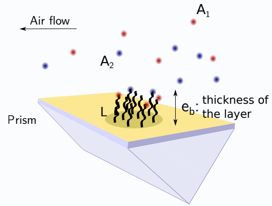

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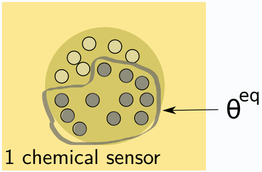
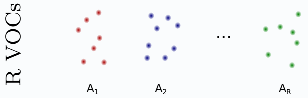


Problem dimensions

Physico-chemical mixture model
Global model

Problem dimensions



Physico-chemical mixture model

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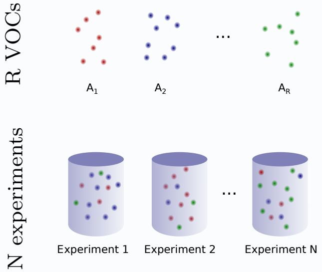

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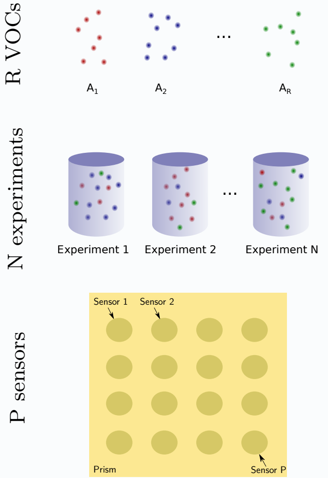

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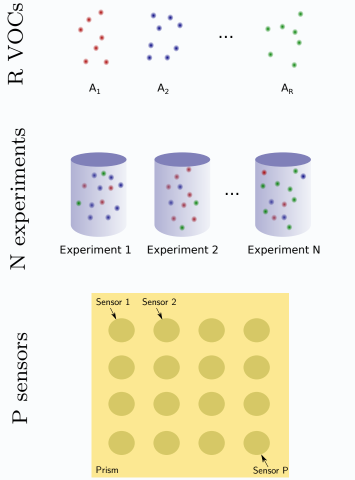


$$y_{pn} = \gamma \frac{\sum_{r=1}^{R} m_r k_{rp} c_{rn}}{1 + \sum_{r=1}^{R} k_{rp} c_{rn}}$$

chemical sensor, mixture → y_{pn}

VOC → m_r

VOC, chemical sensor → k_{rp}

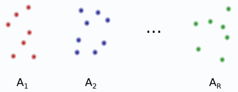
VOC, mixture → c_{rn}

Physico-chemical mixture model

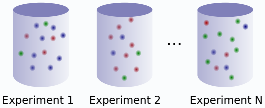
Global model

Problem dimensions

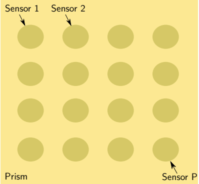
R VOCs



N experiments



P sensors



Matrix formulation

Physico-chemical mixture model
Global model

Problem dimensions

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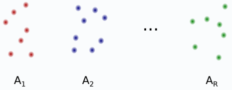

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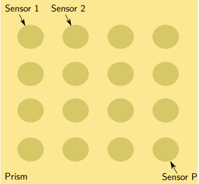
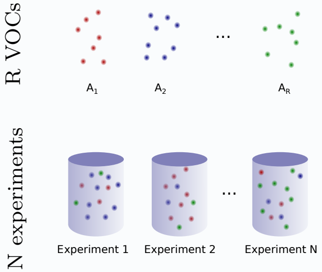


Matrix formulation

$$\underbrace{\begin{bmatrix} \boldsymbol{K} \\ \text{Signat.} \end{bmatrix}}_{R\ \text{VOCs}} \Bigg\} \text{P sensors}$$

Problem dimensions



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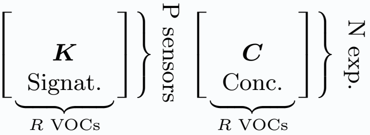

Physico-chemical mixture model

Global model

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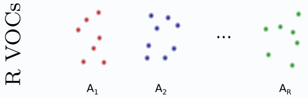


Matrix formulation

$\boldsymbol{K}$ Signat. — P sensors × R VOCs

$\boldsymbol{C}$ Conc. — N exp. × R VOCs

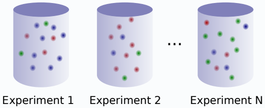
$\boldsymbol{M}$ Masses — R VOCs × R VOCs

$\Downarrow$

Diagonal

Problem dimensions

N experiments



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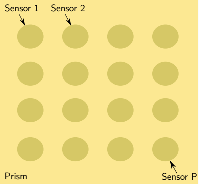

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$\Downarrow$

Diagonal

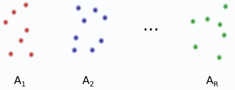
$\boldsymbol{Y}$ Measures: P sensors × N exp.

Physico-chemical mixture model

Global model

Problem dimensions

R VOCs



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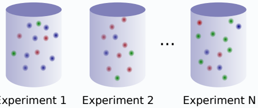

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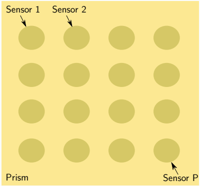

Matrix formulation

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$\boldsymbol{C}$ Conc. — N exp. × R VOCs

$\boldsymbol{M}$ Masses — R VOCs × R VOCs ⇓ Diagonal

$\boldsymbol{Y}$ Measures — P sensors × N exp.

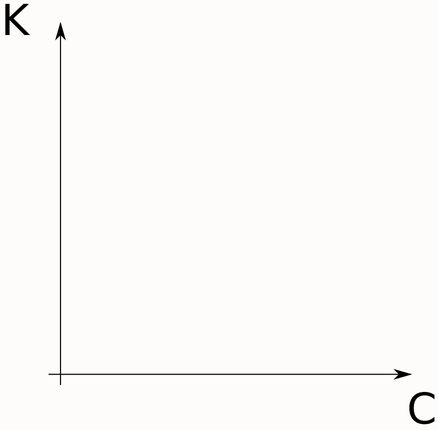
<u>Mixture model</u>

$$\boldsymbol{Y} = \boldsymbol{K}\boldsymbol{M}\boldsymbol{C}^{\mathrm{t}} \oslash (\mathbf{1}_P \mathbf{1}_N^{\mathrm{t}} + \boldsymbol{K}\boldsymbol{C}^{\mathrm{t}})$$

Mixture model

$$\mathscr{L}(\boldsymbol{K},\boldsymbol{C}) = \boldsymbol{Y} = \boldsymbol{K}\boldsymbol{M}\boldsymbol{C}^{\mathrm{t}} \boxslash (\boldsymbol{1}_P\boldsymbol{1}_N^{\mathrm{t}} + \boldsymbol{K}\boldsymbol{C}^{\mathrm{t}})$$

Particular cases



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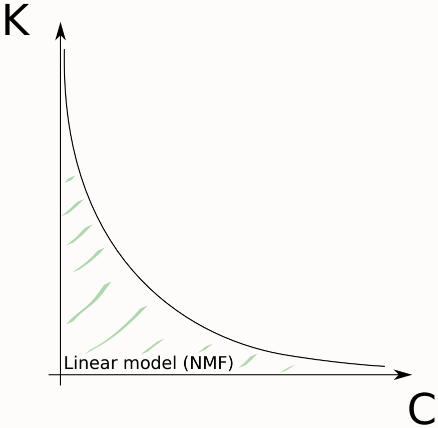
Particular cases

① Low concentration: assuming $\boldsymbol{K}\boldsymbol{C}^{\mathrm{t}} \ll 1$, then

$$\boldsymbol{Y} \approx \boldsymbol{K}\boldsymbol{M}\boldsymbol{C}^{\mathrm{t}}$$

➔ NMF [5]



Mixture model

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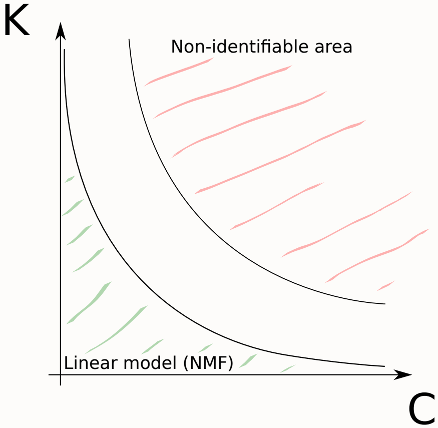
$$\boldsymbol{Y} \approx \boldsymbol{K}\boldsymbol{M}\boldsymbol{C}^{\mathrm{t}}$$

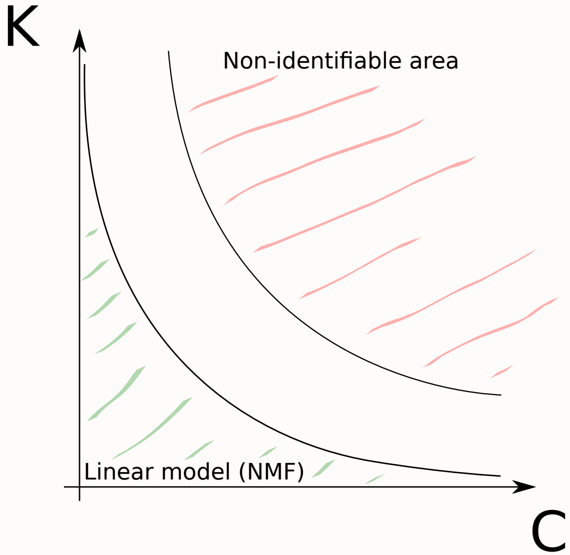
➔ NMF [5]

② Saturation: assuming high concentrations and/or high affinities, then $\boldsymbol{K}\boldsymbol{C}^{\mathrm{t}} \gg 1$

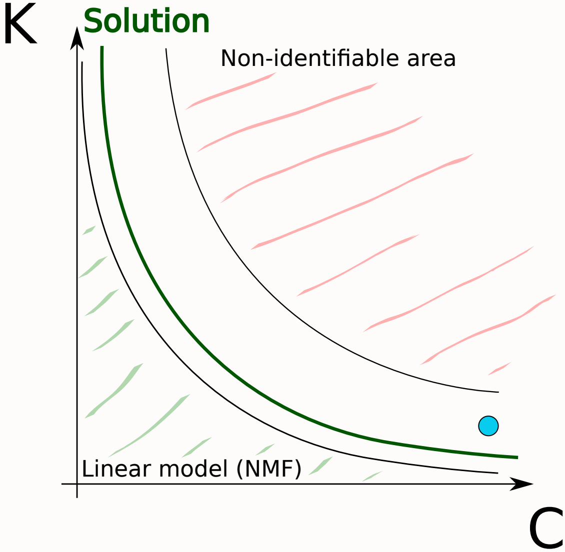
$$\boldsymbol{Y} \approx \boldsymbol{K}\boldsymbol{M}\boldsymbol{C}^{\mathrm{t}} \boxslash \boldsymbol{K}\boldsymbol{C}^{\mathrm{t}}$$

➔ highly non-identifiable:
$\boldsymbol{Y} \approx \boldsymbol{D}_1\boldsymbol{K}\boldsymbol{M}\boldsymbol{C}^{\mathrm{t}}\boldsymbol{D}_2 \boxslash \boldsymbol{D}_1\boldsymbol{K}\boldsymbol{C}^{\mathrm{t}}\boldsymbol{D}_2$

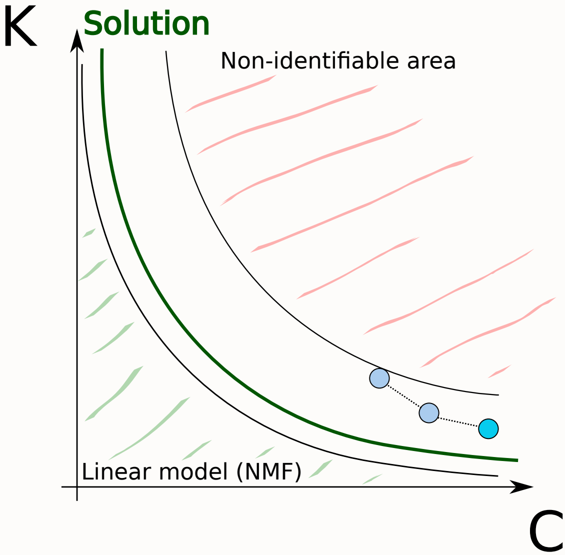


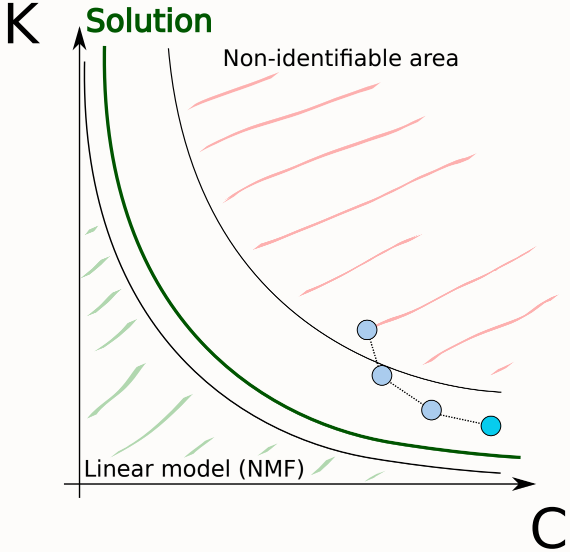


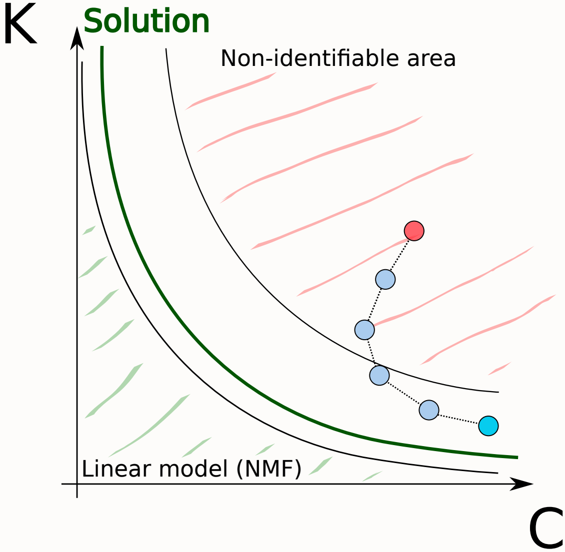
K
Non-identifiable area
Linear model (NMF)
C



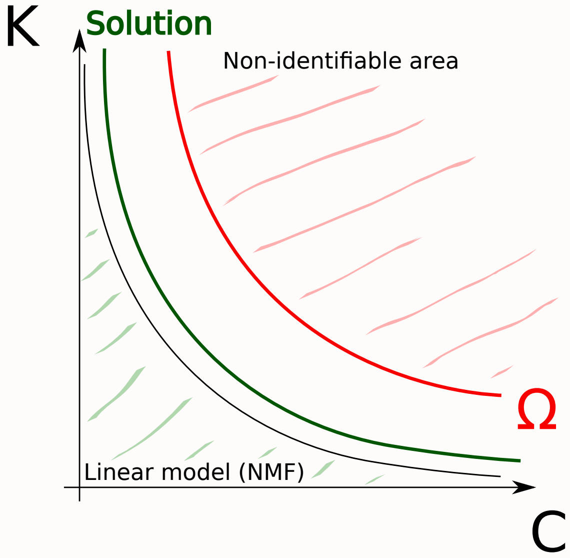
K
Solution
Non-identifiable area
Linear model (NMF)
C

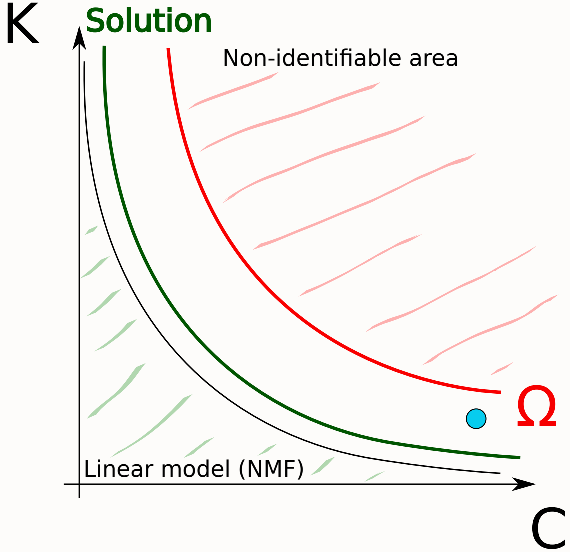

K
Solution
Non-identifiable area
Linear model (NMF)
C

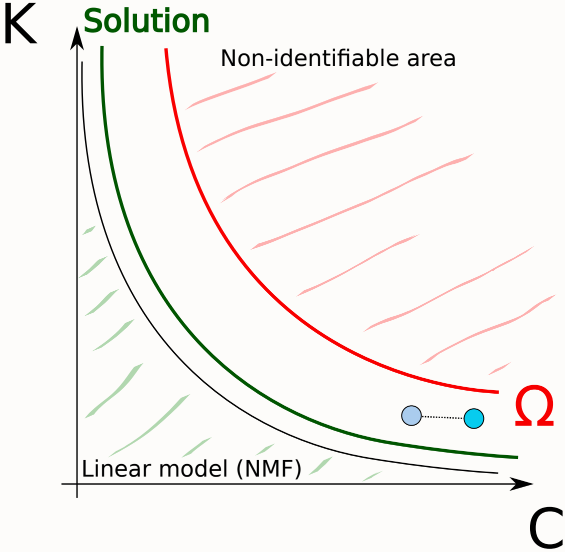

K
Solution
Non-identifiable area
Linear model (NMF)
C

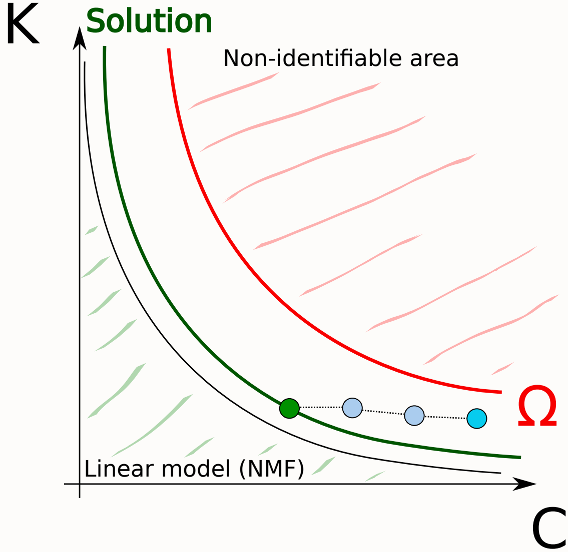


K
Solution
Non-identifiable area
Linear model (NMF)
C


K
Solution
Non-identifiable area
Ω
Linear model (NMF)
C


K
Solution
Non-identifiable area
Ω
Linear model (NMF)
C


K
Solution
Non-identifiable area
Ω
Linear model (NMF)
C


K
Solution
Non-identifiable area
Ω
Linear model (NMF)
C

Definition of Ω

To avoid the saturation area, we can constrain the product $\boldsymbol{KC}$ by :

$$\|\boldsymbol{KC}^{\mathrm{t}}\|_{\max} = R\sup_{ij}((\boldsymbol{KC}^{\mathrm{t}})_{ij}) \leqslant \omega$$

This constraint is not so easy to implement, so we relax it by :

$$\|\boldsymbol{KC}^{\mathrm{t}}\|_{\max} \leqslant \boxed{\|\boldsymbol{K}\|_{\max}\|\boldsymbol{C}^{\mathrm{t}}\|_{\max} \leqslant \omega}$$

Definition of Ω

To avoid the saturation area, we can constrain the product $\boldsymbol{KC}$ by :

$$\|\boldsymbol{K}\boldsymbol{C}^{\mathrm{t}}\|_{\max} = R \sup_{ij}((\boldsymbol{K}\boldsymbol{C}^{\mathrm{t}})_{ij}) \leqslant \omega$$

This constraint is not so easy to implement, so we relax it by :

$$\|\boldsymbol{K}\boldsymbol{C}^{\mathrm{t}}\|_{\max} \leqslant \boxed{\|\boldsymbol{K}\|_{\max}\|\boldsymbol{C}^{\mathrm{t}}\|_{\max} \leqslant \omega}$$

Algorithm

Cost function: $\Upsilon(\boldsymbol{K}, \boldsymbol{C}) = \|\boldsymbol{Y} - \mathscr{L}(\boldsymbol{K}, \boldsymbol{C})\|_F$

Alternating procedure

0 Initialize $\boldsymbol{C}$

1 Estimate $\boldsymbol{K}$ from the sub-problem: $\underset{\boldsymbol{K} \geqslant 0,\ \|\boldsymbol{K}\|_{\max} \leqslant \frac{\omega}{\|\boldsymbol{C}\|_{\max}}}{\arg\min} \Upsilon(\boldsymbol{K}, \boldsymbol{C})$

2 Estimate $\boldsymbol{C}$ from the sub-problem: $\underset{\boldsymbol{C} \geqslant 0,\ \|\boldsymbol{C}\|_{\max} \leqslant \frac{\omega}{\|\boldsymbol{K}\|_{\max}}}{\arg\min} \Upsilon(\boldsymbol{K}, \boldsymbol{C})$

3 Repeat from step 1 until convergence

Simulation results

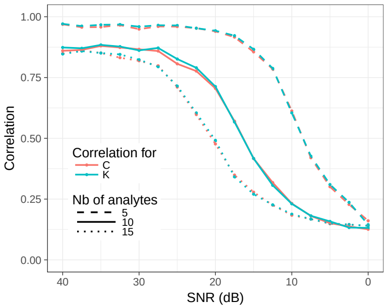
Simulation settings

R VOCs	5/10/15
N experiments	100
P sensors	100

Data are simulated with an additional gaussian noise: $\boldsymbol{Y} = \mathscr{L}(\boldsymbol{K}, \boldsymbol{C}) + \boldsymbol{\epsilon}$ with $\epsilon_{ij} \sim \mathcal{N}(0, \sigma_n)$

The noise is progressively intensified by decreasing the following Signal to Noise Ratio (SNR):

$\text{SNR} = 20 \log(\frac{\sigma_s}{\sigma_n})$ with $\sigma_s = \sqrt{\frac{\|\boldsymbol{Y}\|_2^2}{PN}}$



Conclusion

We have

① formulated a non-linear mixture model for a type of chemical sensors used in an electronic nose.

② proposed an algorithm in order to estimate blindly the individual outputs and the concentrations.

③ assessed the performance of the algorithm in the presence of noise.

Further work will

① include experiments with real data.

② relax the assumption that we know the masses.

③ exploit time information.

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Thank you ! Questions ?