An Overview of Signal Processing Issues in Chemical Sensing

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Outline

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SP in Analytical Chemistry

- Analytical chemistry: to study physical and chemical properties of natural or artificial materials
  - Qualitative analysis: what compound is present? (detection)
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Many things in common with Signal Processing!

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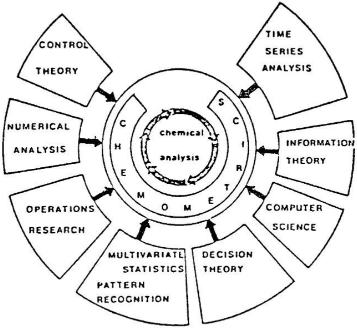

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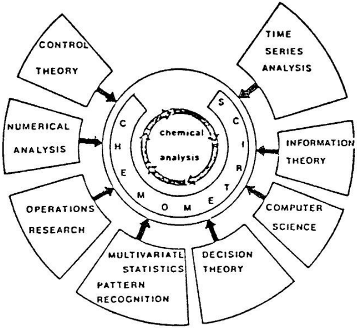

- From www.udel.edu/chemo/Links/chemo_def.htm
- Adapted from B. G. M. Vandeginste, Analytica Chimica Acta, 150 (1983) 199-206.

Common methods in Chemometrics

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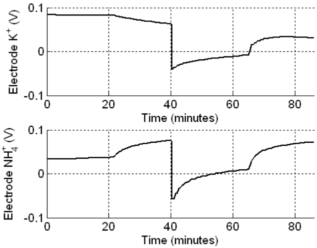
- Savitsky-Golay filter
  - Smoothing filter
  - One of most cited work in analytical chemistry
  - Recently discussed in a IEEE SP Magazine paper (Schafer, 2011)

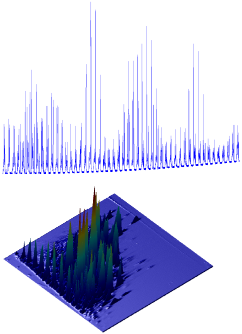
Outline

Chemical data

- Not too different than what we are used to in SP
- Non-negative, sparse, smooth, multidimensional, etc
- Problem: often only a few samples are available



(a) Sensor array.



(b) Gas chromatogram.

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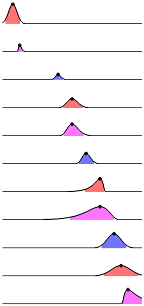

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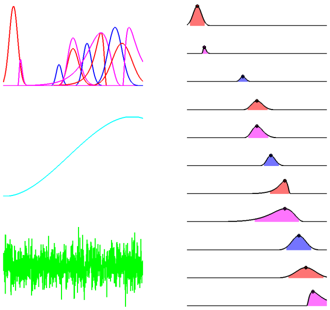
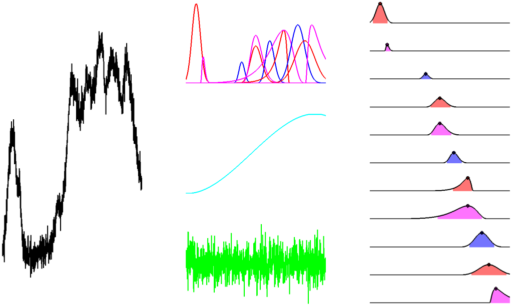


Background estimation and filtering

- What does the analytical chemist want?
  - areas & locations $\Leftrightarrow$ (quantities) of (chemical species)
  - $\pm$ additive mixture: different peaks, background, noise
  - to be dealt with few parameters (one at most)



- Automated background and filtering still required

Acquisition and Compression Problems

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  - Reduction in acquisition time is fundamental in some analysis
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- Compressive sensing
  - Acquisition and compression are conducted at the same time
  - Example of application: NMR spectroscopy (Holland et al., 2011)

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Sensor array processing

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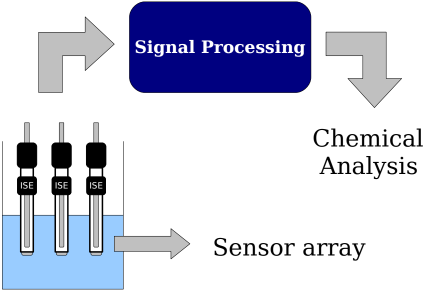
- More recent approach: sensor arrays



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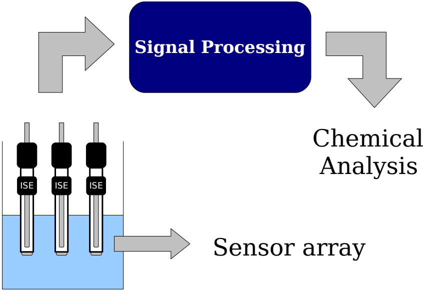
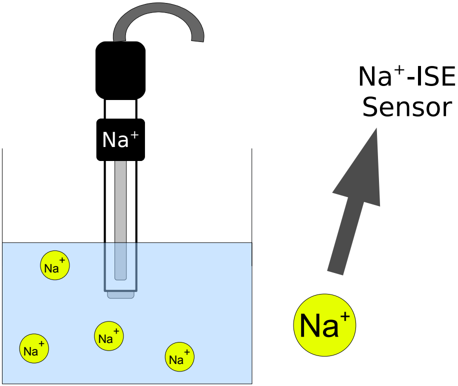


- Flexibility
- Adaptability
- Robustness
- Low cost
- Multi-component analysis

Selectivity issues

- Example: ion-selective electrodes.
- Major inconvenient of an ISE is the lack of selectivity.



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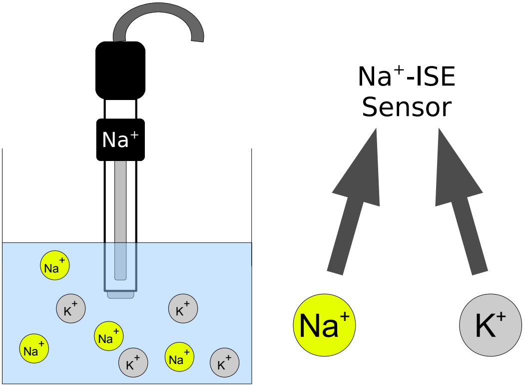
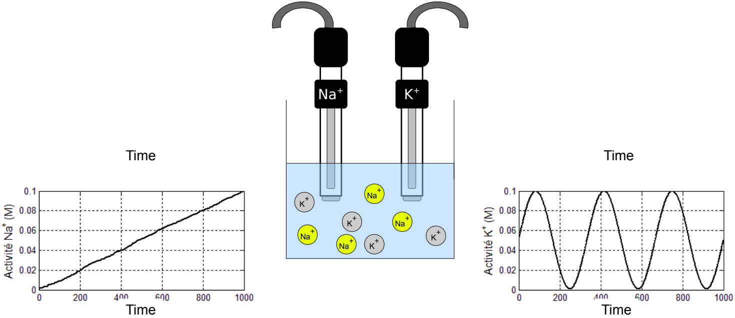


- **There is an interference issue here!**

Sensor array based on blind source separation

- **Sources**: temporal evolution of the ionic activities

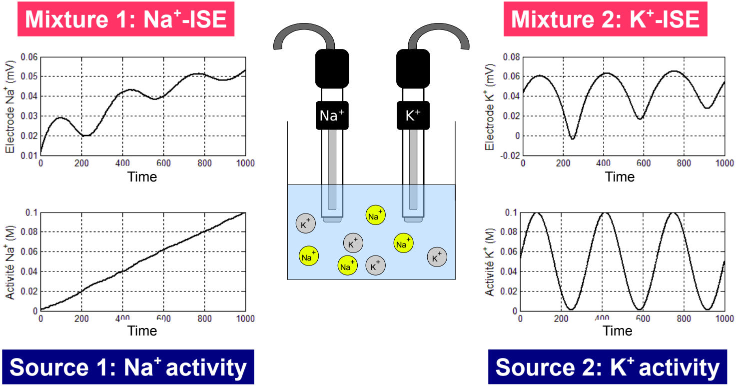


Source 1: Na^+ activity

Source 2: K^+ activity

Sensor array based on blind source separation

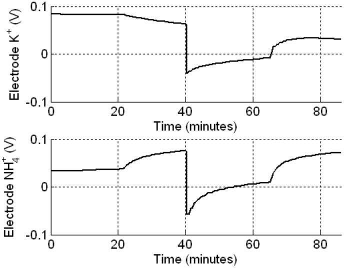
- **Sources**: temporal evolution of the ionic activities
- **Mixtures**: sensors response



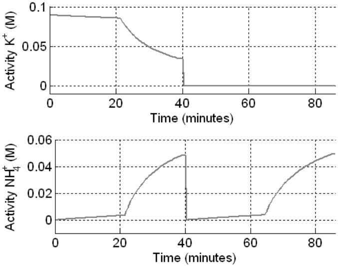
- **The goal is to estimate the ionic activities by only using the mixed signals.**

Example with actual data

- Separation of K^+ and NH_4^+ activities
- Difficulties: Nonlinear mixing model and dependent sources (Duarte et al., 2009)



(a) ISE array response.



(b) Actual sources.

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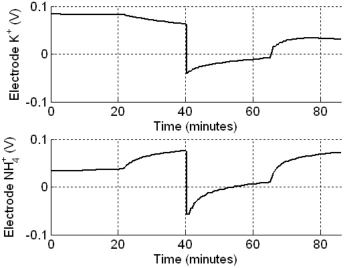

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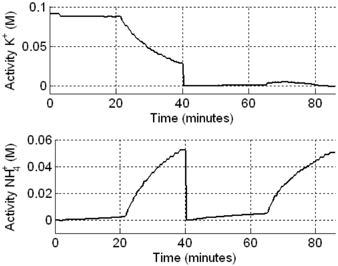
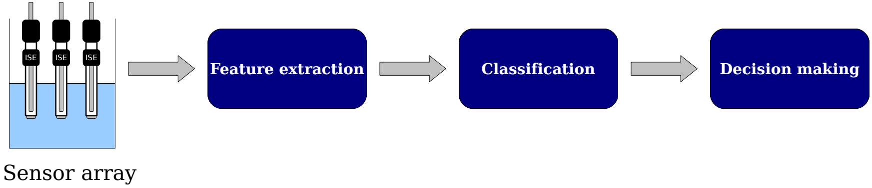


(b) Retrieved sources.

Machine learning: Electronic noses and tongues

- Automatic odor and taste pattern recognition by exploiting diversity
- Some applications:
  - Food and beverage analysis
  - Environmental monitoring
  - Disease diagnosis



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An overview on the Special Session

- Different applications and methods are addressed.

1. *Primal-dual interior point optimization for a regularized reconstruction of NMR relaxation time distributions*
   - E. Chouzenoux, S. Moussaoui, J. Idier, F. Mariette
   - **Non-negativity, NMR spectroscopy, optimization.**
2. *Sparse modal estimation of 2-D NMR signals*
   - Souleymen Sahnoun, El-Hadi Djermoune, David Brie
   - **Non-negativity, sparsity, NMR spectroscopy.**
3. *Active analysis of chemical mixtures with multi-modal sparse non-negative least squares*
   - Jin Huang, Ricardo Gutierrez-Osuna
   - **Non-negativity, sparsity, Infra-red sensors.**
4. *Recursive least squares algorithm dedicated to early recognition of explosive compounds thanks to multi-technology sensors*
   - Aurélien Mayoue, Aurélie Martin, Guillaume Lebrun, Anthony Larue
   - **Classification, RLS algorithm, Multidimensional analysis, E-nose.**

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Conclusions

- Analytical chemistry is an interesting field of application for signal processing methods
- Possible interaction between the two domains is very wide
- Insights from chemists are very important
- The main goal of this special session is to draw the signal processing community attention to these new possibilities

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