ARTIFICIAL CHEMICAL SENSES - ELECTRONIC TONGUE & ELECTRONIC NOSE

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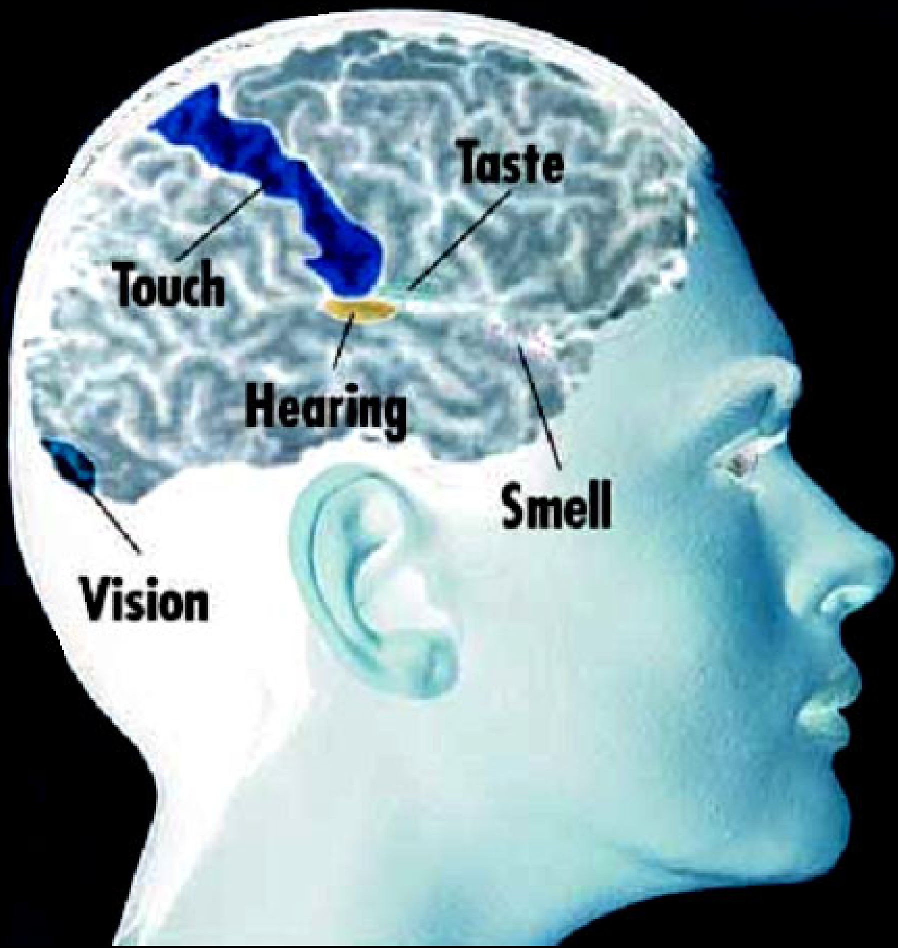
CSRG

Human senses



- Physical
  - Vision
  - Hearing
  - Touch
- Chemical
  - Smell
  - Taste

Bionics

- ↗ study
- ↗ modeling
- ↗ analysis

Of functioning of biological organisms

↗Construction of analogous functioning devices

- Fusion of biological and artificial organs => implants, biomaterials...
- devices simulating biological constructions and systems => artificial kidney, electronic tongue....

↗For theoretical-cognitive orders

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ELECTRONIC TONGUE / ELECTRONIC NOSE (ETongue, ENose)

- systems for automatic analysis and recognition (classification) of liquids or gases
- Electronic tongues - **liquid** samples
- Electronic noses – **gaseous** samples
- The result of analysis: the identification of the sample, an estimation of its concentration or its characteristic properties
- many advantages: problems associated with human senses, like individual variability, impossibility of on-line monitoring, subjectivity, adaptation, infections, harmful exposure to hazardous compounds, mental state, are no concern of it.
- Synonyms: artificial tongue, taste sensor, artificial nose, olfactory system

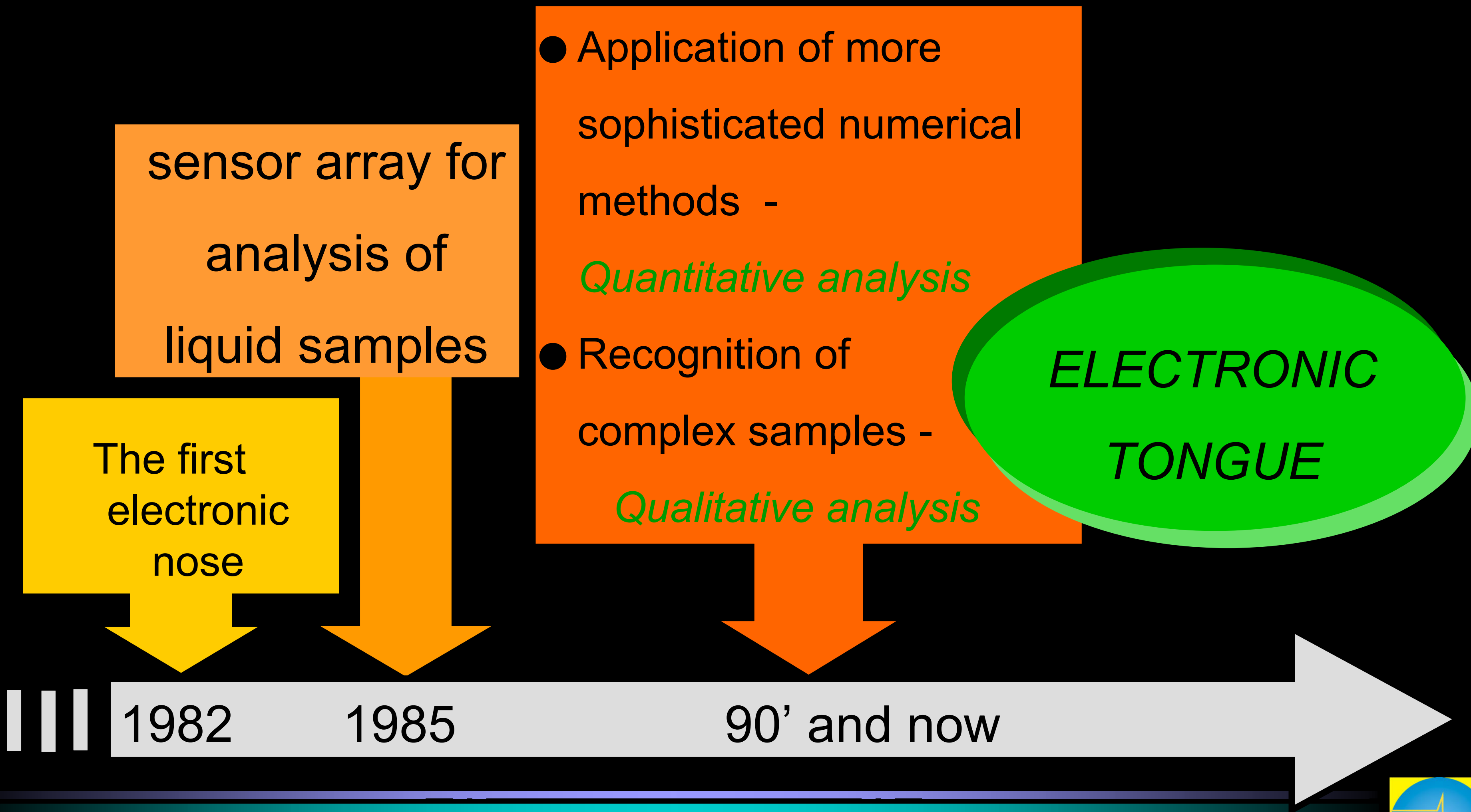
Electronic tongue / Electronic nose

A SYSTEM FOR AUTOMATIC ANALYSIS AND CLASSIFICATION (RECOGNITION) OF SAMPLES

AN ARRAY OF CHEMICAL SENSORS

PATTERN RECOGNITION SYSTEM

Sensor arrays



Applications

Foodstuffs Industry

- food quality control during processing and storage (water, wine, coffee, milk, juice…)
- optimization of bioreactors
- control of ageing process of cheese, whiskey
- automatic control of taste

Medicine

- non-invasive diagnostics (patient's breath, analysis of urine, sweat, skin odour)
- clinical monitoring in vivo
- identification of unpleasant odour of pharmaceuticals

Quality control of air in buildings, closed accommodation (i.e. space station, control of ventilation systems)

Applications

Safety

- searching for chemical/biological weapon
- searching for drugs, explosives
- friend-or-foe identification

Environmental pollution monitoring

- monitoring of agricultural and industrial pollution of air and water
- identification of toxic substances
- leak detection

Chemical Industry

- products purity
- in the future - detection of functional groups, chiral distinction

Legal protection of inventions - digital "fingerprints" of taste and odours

SENSING METHODS APPLIED

- Potentiometric sensors
- Measurements of conductivity
- Voltamperommetry
- Optical sensors
- Biosensors

E-TONGUE

- Conductivity sensors (MOSFET, CP)
- Piezoelectric sensors (QMB, SAW)
- Optical sensors

E-NOSE

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Pattern recognition

The electronic tongue or nose system performance is dependent on the **quality of functioning of its pattern recognition block**. Various techniques and methods can be used separately or together to perform the recognition of the samples. After measurement procedure the signals are transformed by a **preprocessing block**. The results obtained are inputs for **Principal Components Analysis**, **Cluster Analysis** and/or **Artificial Neural Network**.

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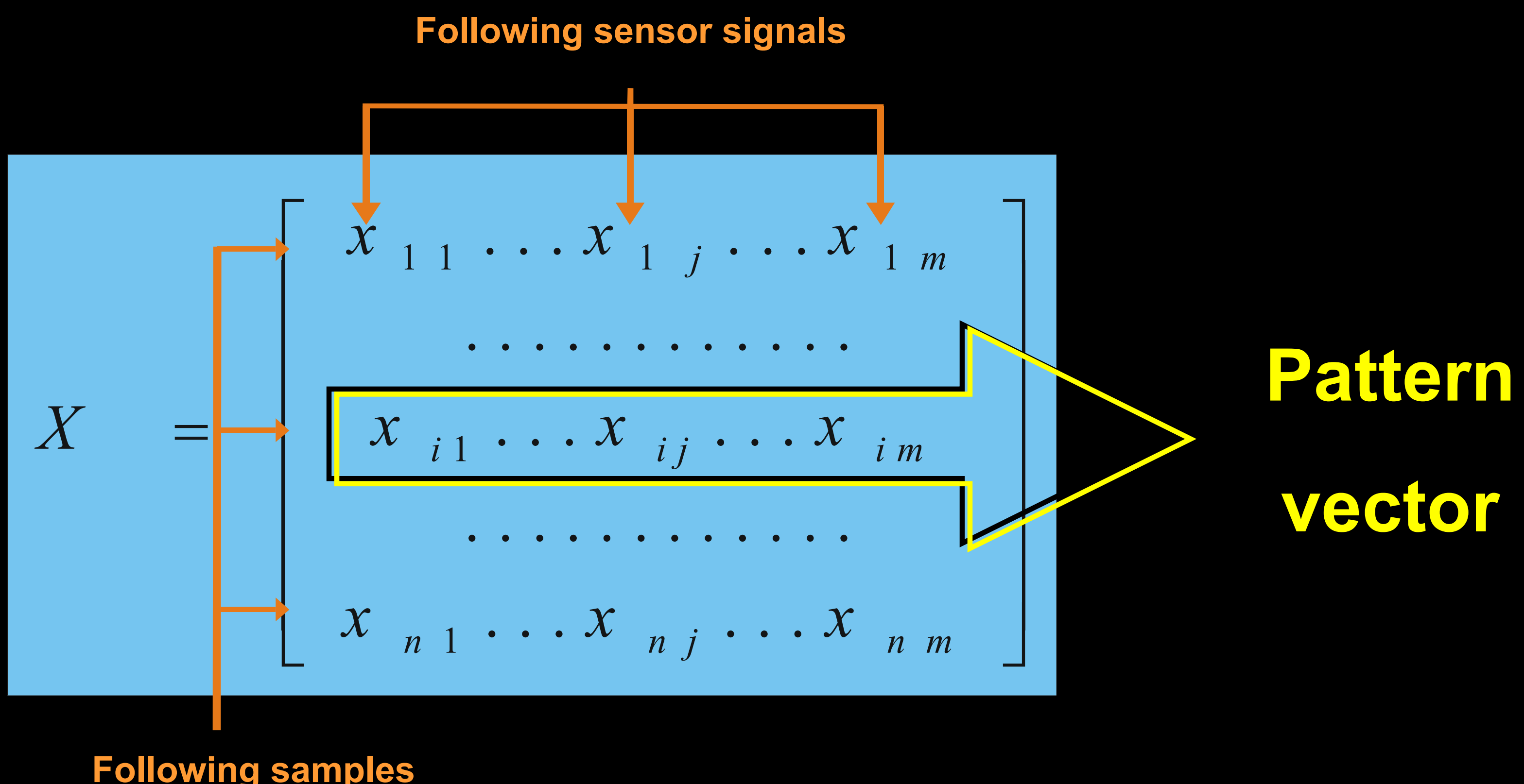
Data Analysis - **Data matrix**

- Each sample is characterized by unique and typical set of data, forming "fingerprint" of an analyte in m-dimensional pattern space.

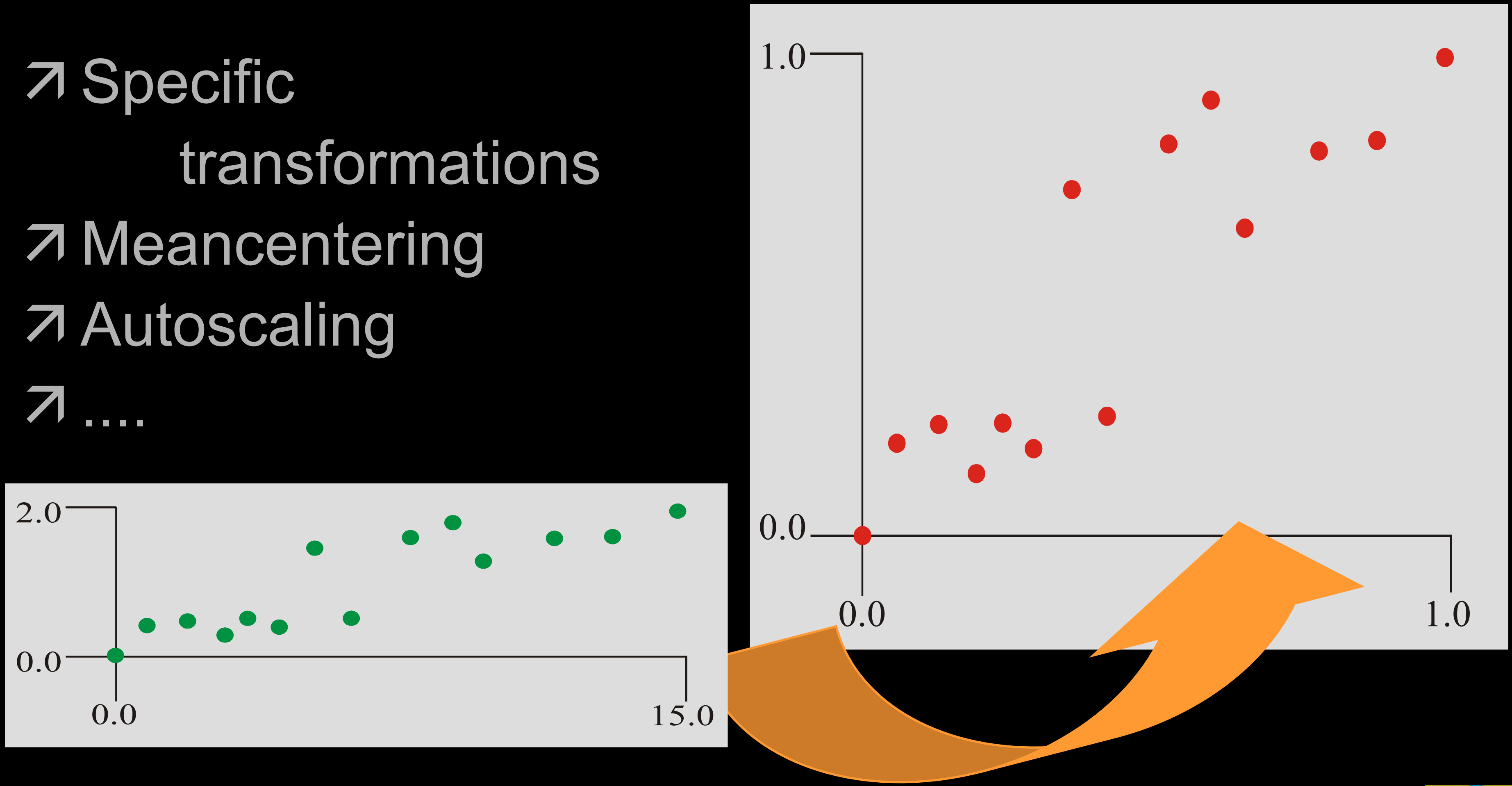


Data Analysis - **Preprocessing**

- linear transformation on the data matrix is performed (without changing the dimensionality of the problem) in order to enhance qualitative information.
- Typical techniques: manipulation of sensor baseline, normalization, standarization and scaling of response for all the sensors in an array.

Data Analysis - **Preprocessing**

- Specific transformations
- Meancentering
- Autoscaling
- ....



Principal Components Analysis and Cluster Analysis

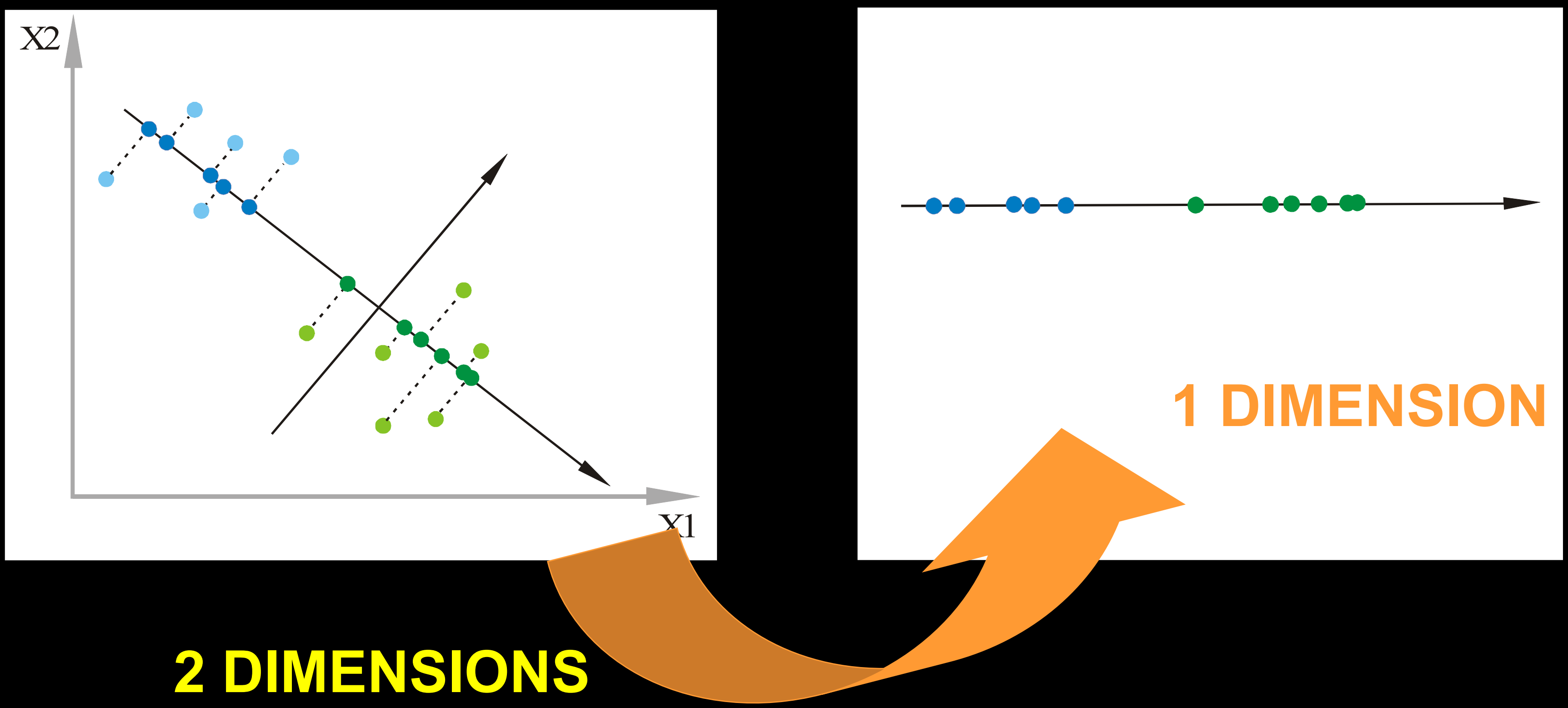
- A multi-sensor system produces data of **high dimensionality** - hard to handle and visualize
- **Principal Component Analysis** (PCA) and **Cluster Analysis** (CA) are multivariate pattern analysis techniques reducing dimensionality of the problem and reducing high degree of redundancy.

Principal Components Analysis (PCA)

linear feature-extraction technique finding most influential, new directions in the pattern space, explaining as much of the variance in the data set as possible.

This new directions - called principal components - are the base for a new data matrix. Usually 2 or 3 of them are sufficient to transfer more than 90% of the variation of the samples.

Data Analysis –
Principal Component Analysis (PCA)



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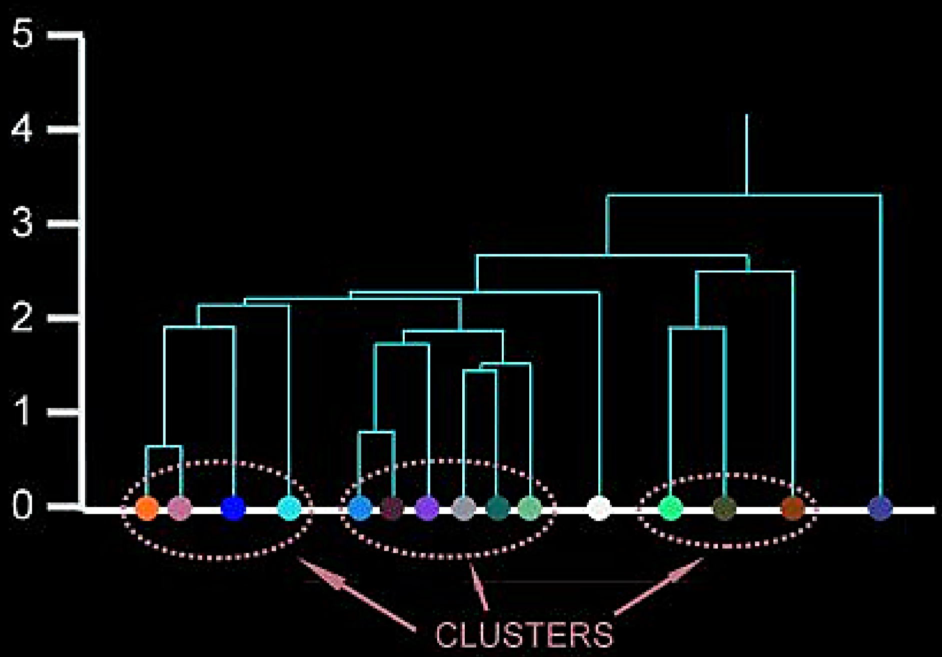
Cluster Analysis (CA)

The base principle of Cluster Analysis is the assumption of close position of similar samples in multidimensional pattern space.



Similarity between each 2 samples is calculated as a function of the distance between them - usually in Euclidean sense - and displayed on a dendrogram.

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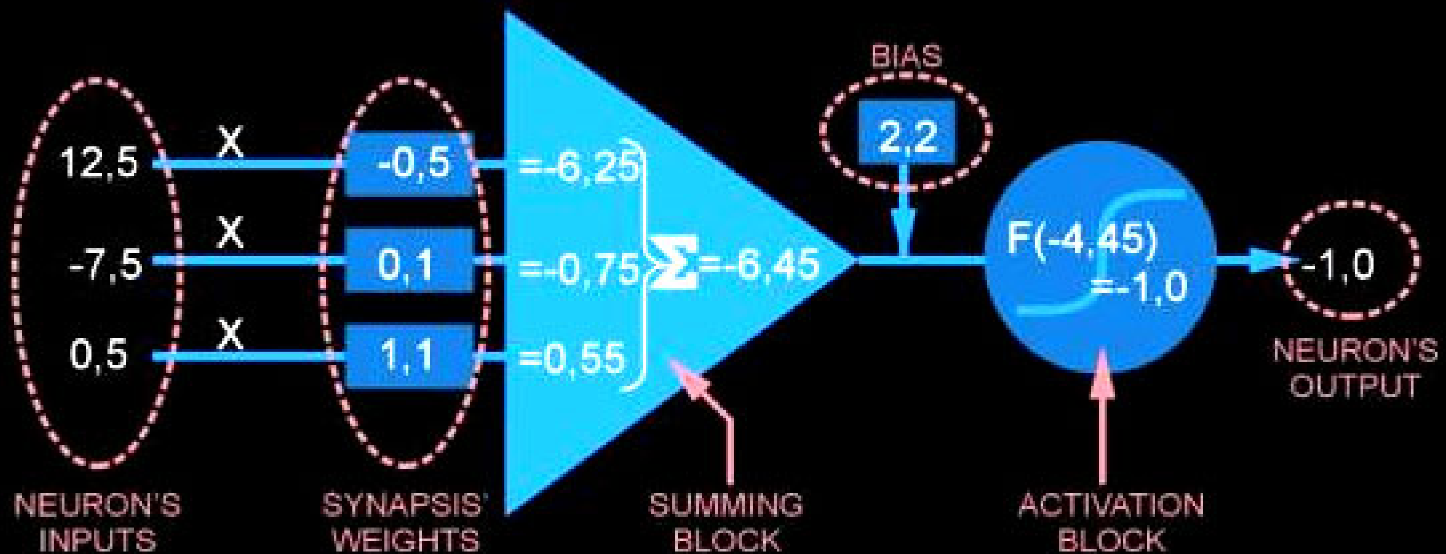
Artificial Neural Network (ANN)

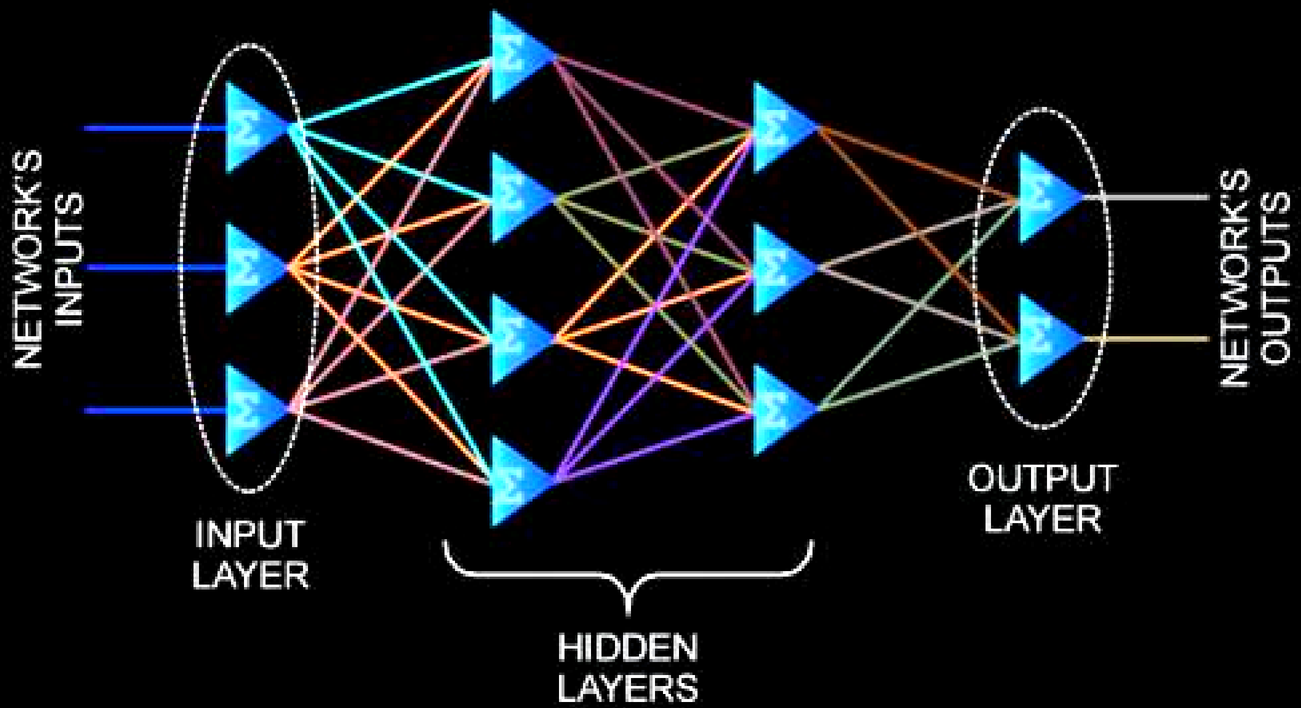
- information processing structures imitating behaviour of human brain
- main advantages: adaptive structure, complex interaction between input and output data, ability to generalize, parallel data processing and handling incomplete or high noise level data =>useful pattern recognition tool
- many possible architectures and algorithms available in the literature
- the most common in measurement applications is feed-forward network and back-propagation learning algorithm.

Artificial Neural Network (ANN)

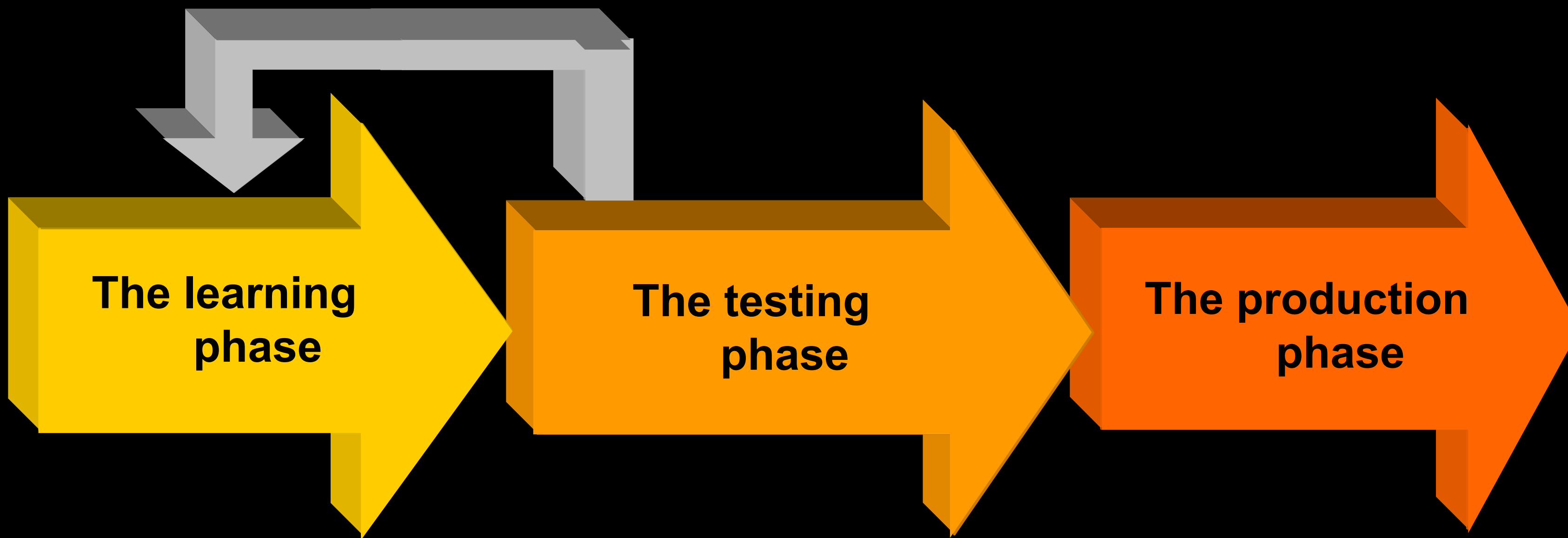


The base units of artificial neural networks are neurons and synapses. Neurons are organized in layers and connected by synapses. Their task is to sum up their inputs and non-linear transfer of the result, which is then transmitted via synapsis with modification by means of the synapsis weights - this signal, in turn, is the input for the next layer of the network

Artificial Neural Network (ANN)



Artificial Neural Network (ANN)



- ↗ network is forced to provide desired outputs corresponding to a determined input
- ↗ adjusting the synapses' weights

✓verification of the generalization capability of network

✓network is capable of providing outputs corresponding to any input

Electronic tongue developed at Warsaw University of Technology

Sensor array

Ion-selective electrodes (ISEs)

- Selective
- Partially selective

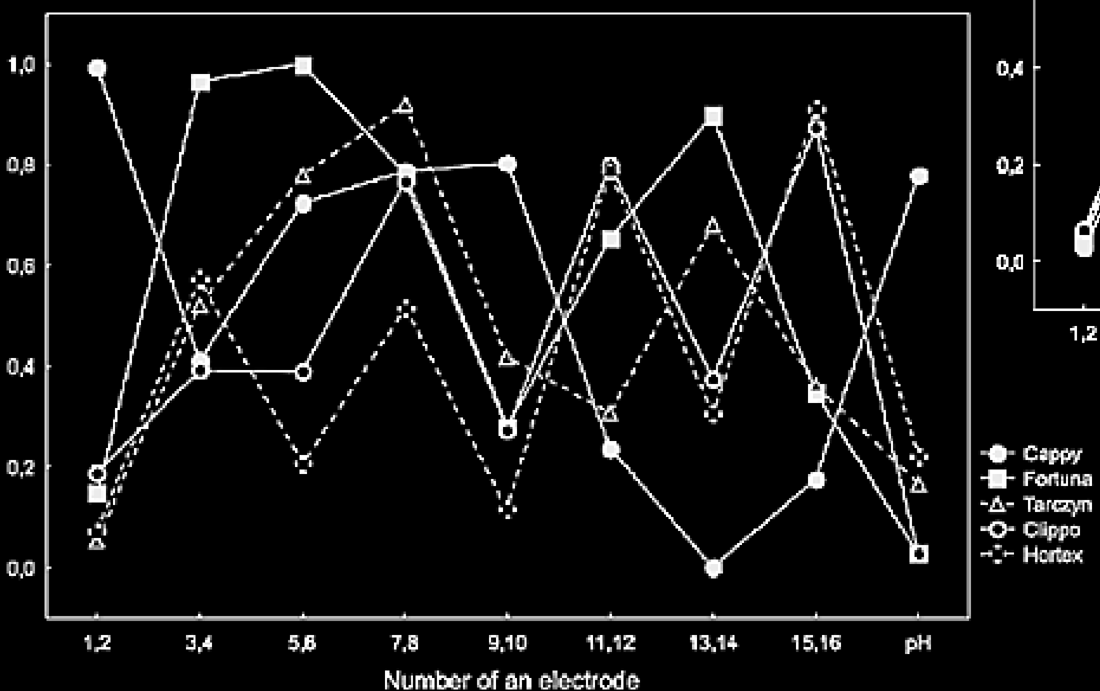
Data analysis

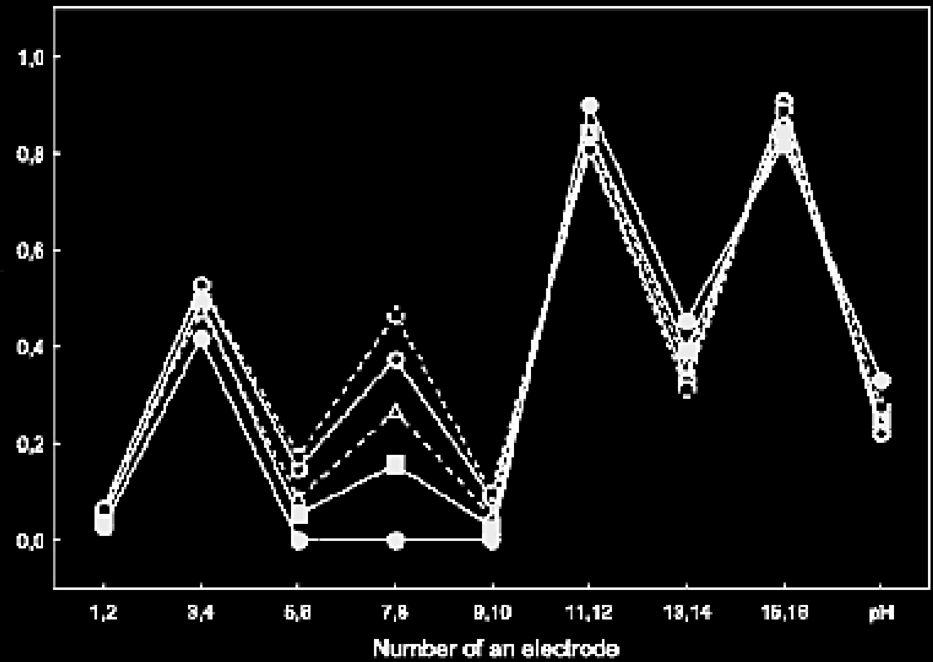
- Extraction of information from multidimensional measurement data

- PCA
- ANN
- SIMCA (Soft Independent Modeling of Class Analogy)
- PLS (Partial Least Squares)
- More...

Juice brand recognition

All brands

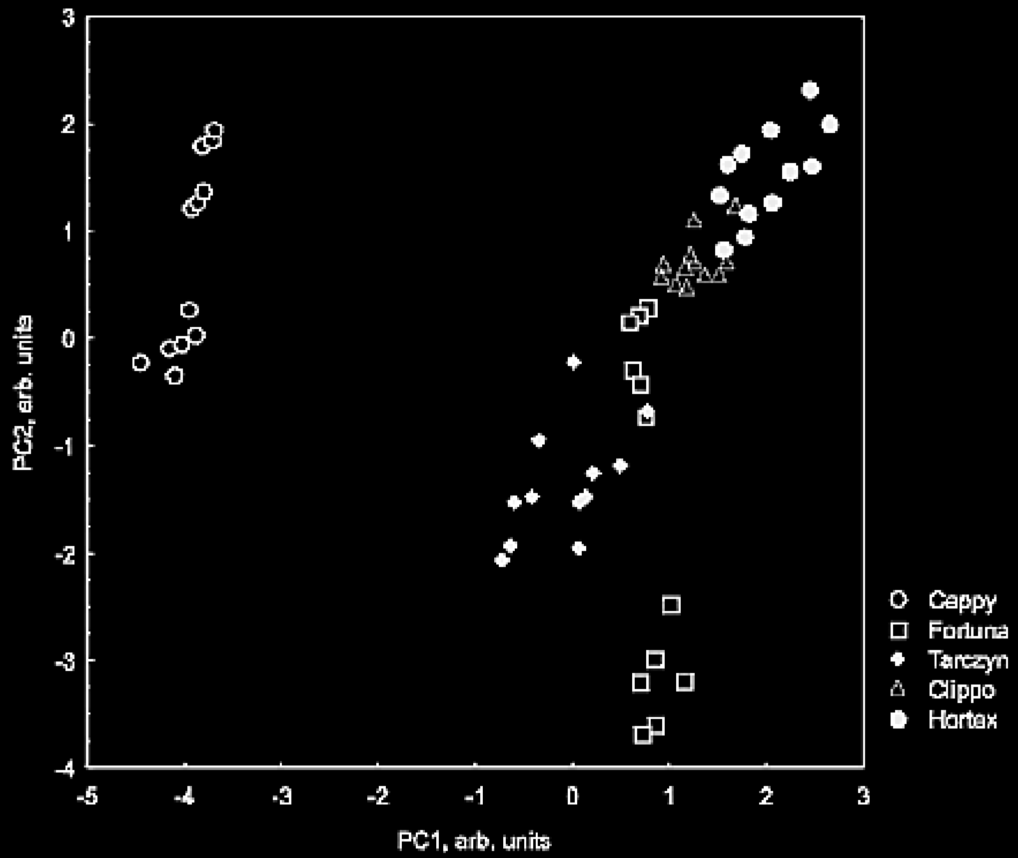




One brand

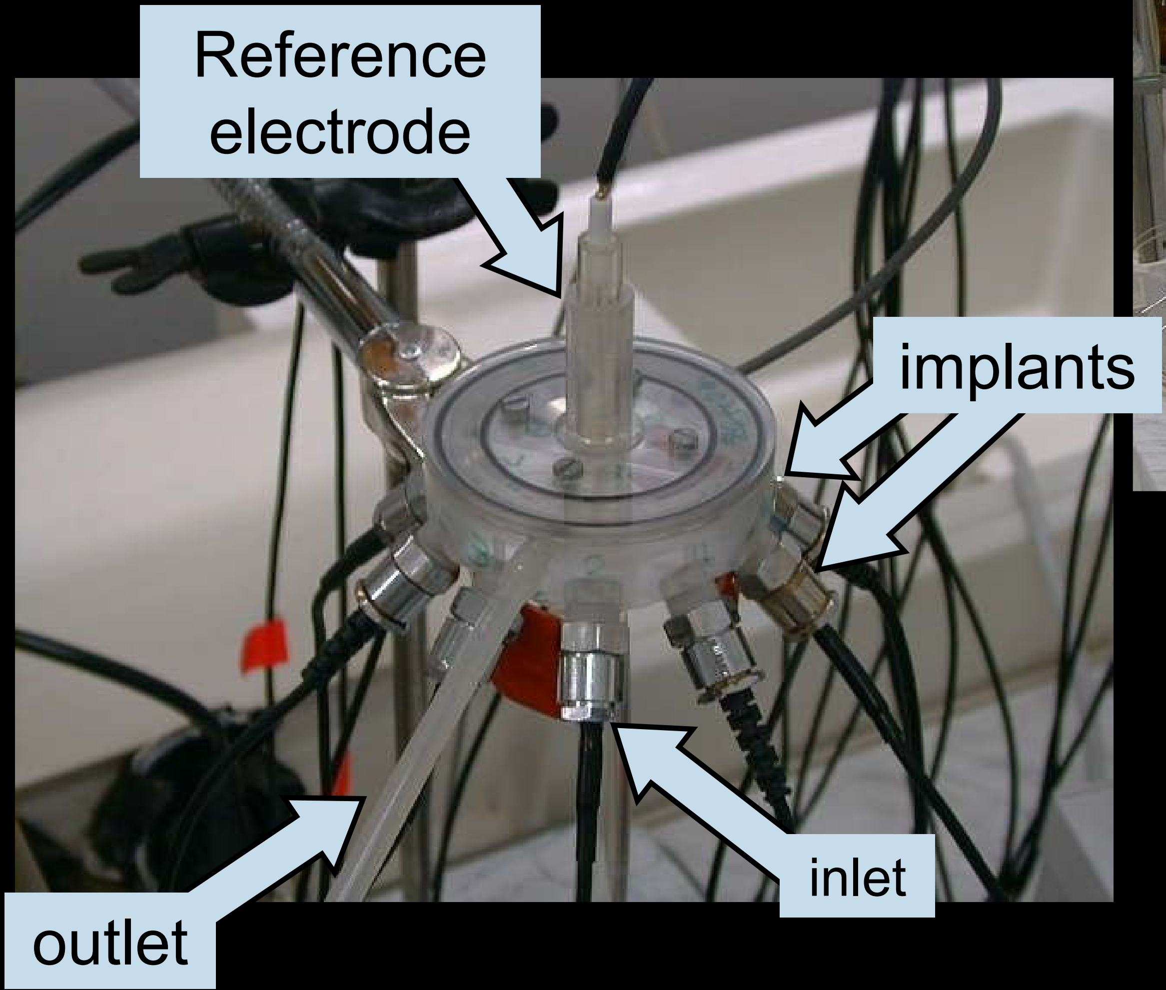
(Hortex)

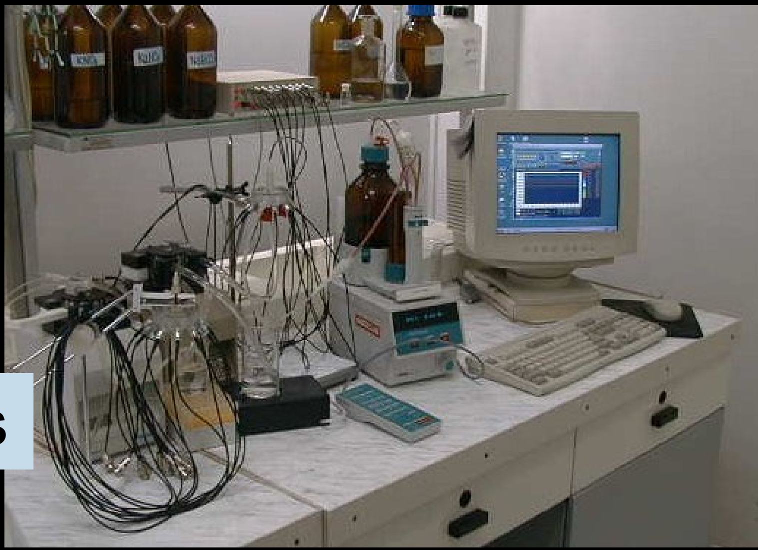
Juice measurements – PCA & ANN



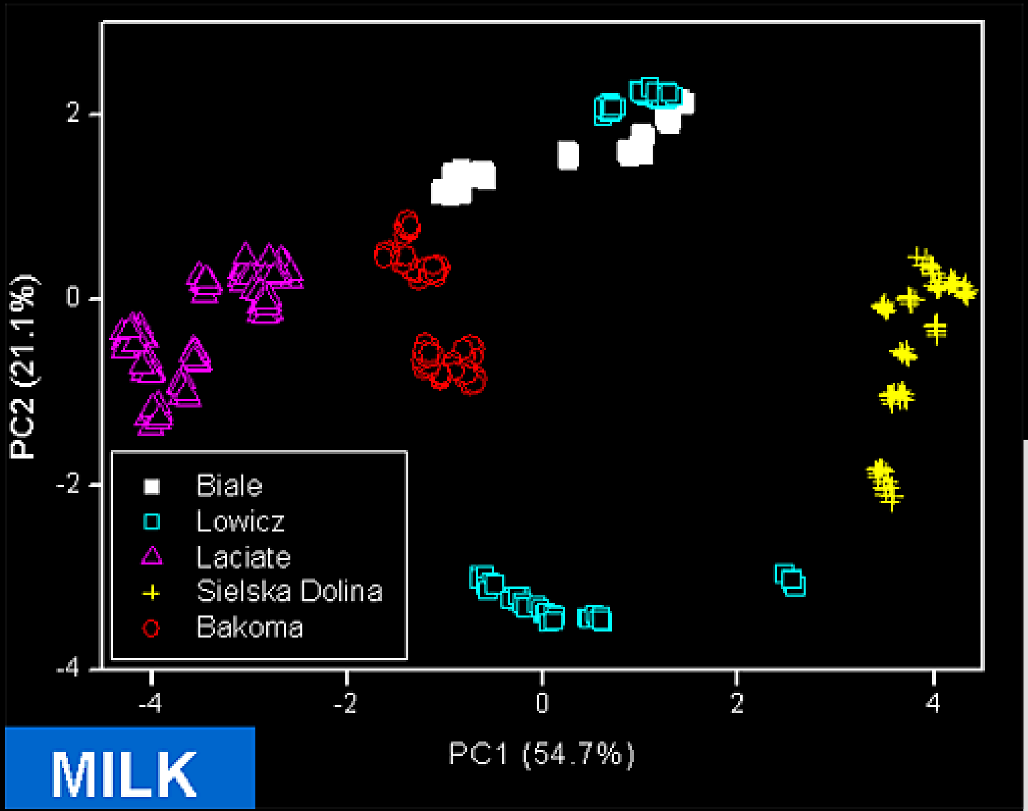
- **Mean squared error of neural net processing** 3.09 * 10^{-4}
- **% of correct classifications** 92.0

Miniaturized flow-through electronic tongue





Beverages recognition



	% of correct classifications
Orange juice	86,7
Milk	96,7
Beer	86,3

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Commercial Systems

- Aromascanner (Aromascan, UK)
- Fox Intelligent Nose (Alpha MOS, France)
- Taste sensing system SA401 (Anritsu Corp., Japan)

cost :

20 000 – 100 000 $

Comparison of natural and artificial chemical senses

Natural	Artificial
Sample delivery - periodical	Sample delivery - continuous
Receptors ↗Non-selective ↗High redundancy ↗Biochemical transduction ↗Signal: pattern of spikes	**Sensors** ↗Selective/partially selective ↗Low redundancy ↗Chemical transduction ↗Signal: steady signal
Signal processing – data synthesis	Signal processing – one sensor – one signal
Data analysis ↗Wide database ↗High integration with other senses	**Data analysis** ↗Limited database ↗Possible to integrate with other instruments (for example fusion of e-tongue&e-nose)

References

1. P. Ciosek, Z. Brzózka, W. Wróblewski, Classification of beverages using a reduced sensor array, Sens. Actuators B, 103 (2004), 76-83.
2. P. Ciosek, E. Augustyniak, W. Wróblewski, Polymeric membrane ion-selective and cross-sensitive electrodes-based electronic tongue for qualitative analysis of beverages, Analyst, 129 (2004), 639-644.
3. P. Ciosek, Z. Brzózka, W. Wróblewski, E. Martinelli, C. Di Natale, A. D'Amico, Direct and two stage data analysis procedures based on PCA, PLS-DA and ANN for ISE-based electronic tongue – effect of supervised feature extraction, Talanta, in press
4. P. Ciosek, W. Wróblewski, The analysis of sensor array data with various pattern recognition techniques, Sens. Actuators B, in press
5. D'Amico A., Di Natale C., Paolesse R., Portraits of gasses and liquids by arrays of nonspecific chemical sensors: trends and perspectives, Sensors and Actuators B, 68 (2000), 324
6. Toko K., Taste sensors with global selectivity, Materials Science and Engineering, C4 (1996), 69
7. Vlasov Y., Legin A., Non-selective chemical sensors in analytical chemistry: from "electronic nose" to "electronic tongue", Journal of Analytical Chemistry, 361 (1998), 255
8. Krantz-Ruckler C., Stenberg M., Winquist F., Lundstrom I., Electronic tongues for environmental monitoring based on sensor arrays and pattern recognition: a review, Analytica Chimica Acta, 426 (2001), 217
9. Winquist F., Holmin S., Krantz-Ruckler C., Wide P., Lundstrom I., A hybrid electronic tongue, Analytica Chimica Acta, 406 (2000), 147

Links

Commercially available e-noses/e-tongues:

- http://www.alpha-mos.com/
- http://www.detect-measure.com/neo.htm
- http://www.osmetech.plc.uk/
- http://www.appliedsensor.com/
- http://www.airsense.com
- http://cyranosciences.com/
- http://estcal.com/
- http://www.hkr-sensor.de/
- http://www.lennartz-electronic.de/

Chemometrics:

- http://ull.chemistry.uakron.edu/chemometrics/
- http://www.spectroscopynow.com/Spy/basehtml/SpyH/1,1176,2-0-0-0-0-home-0-0,00.html/

Summary

- Novel method in chemical analysis
- Application of chemometrics, mathematics, statistics, artificial intelligence
- Elimination of subjective, human estimation

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