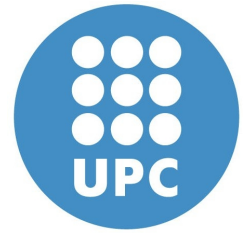


Centre de Recerca en Enginyeria Biomèdica

Universitat Politècnica de Catalunya

PhD Thesis in Biomedical Engineering

Biomimetic set up for chemosensor-based machine olfaction

Aspirant: Andrey Ziyatdinov

Adviser: Alexandre Perera i Lluna

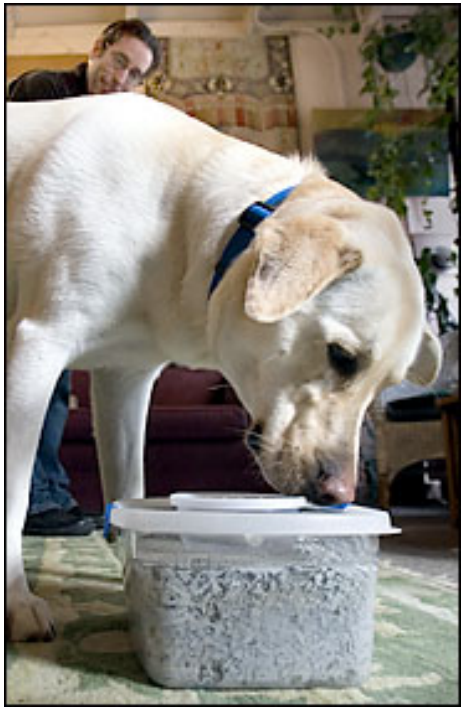
4 December, 2014

Outline

A story from NYT

The New York Times
Dogs Excel on Smell Test to Find Cancer
By Donald G. McNeil Jr., 2006

Five dogs were trained to detect lung cancer in the breath of patients (N = 138) with 99 % accuracy [McCulloch et al., 2006]



Kobi in a cancer-detection experiment

Keys to success

- Known biomarkers are volatile organic compounds, e.g. alkanes
- Dogs detect odors in the very low parts-per-billion (ppb) range
- 'Pattern recognition' by means of the canine olfactory system

An engineering solution

The colorimetric sensor array consisted of 36 chemically sensitive dots (e.g. metalloporphyrins) impregnated on a disposable cartridge.

A moderate accuracy of a random forest classifier with 73 % sensitivity and 72 % specificity (N = 143) [Mazzone et al., 2007]

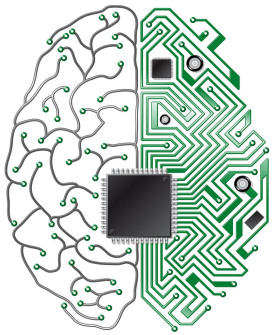
36 chemically sensitive spots

System principles

- 36 composites were selected to be generally responsive
- Such systems perform at up to ppb range for specific volatiles
- The identity of the key VOCs has not been clearly established
- Hypothesis: an array is able to detect the unique pattern of VOCs

Biomimetic context

Biomimetic set up

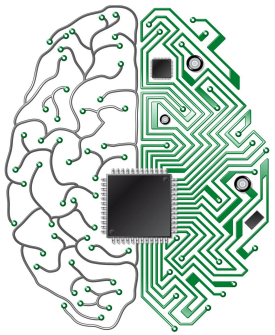


Trained dogs

Chemosensors

Biomimetic context

Biomimetic set up



Biomimetic neural learning

High-dimensional sensory input

Smell fingerprint

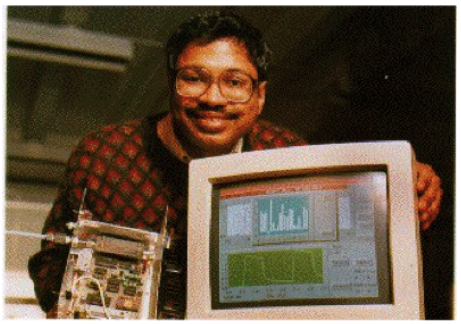
Trained dogs

Chemosensors

First proposal

First proposed by Krishna Persaud and George Dodd in 1982 [Persaud and Dodd, 1982]

> "... we suggest that to make fine discriminations between complex odorant mixtures containing varying ratios of odorants without the necessity for highly specialized peripheral receptors, the olfactory systems makes use of feature detection using broadly tuned receptor cells organized in a convergent neuron pathway. "



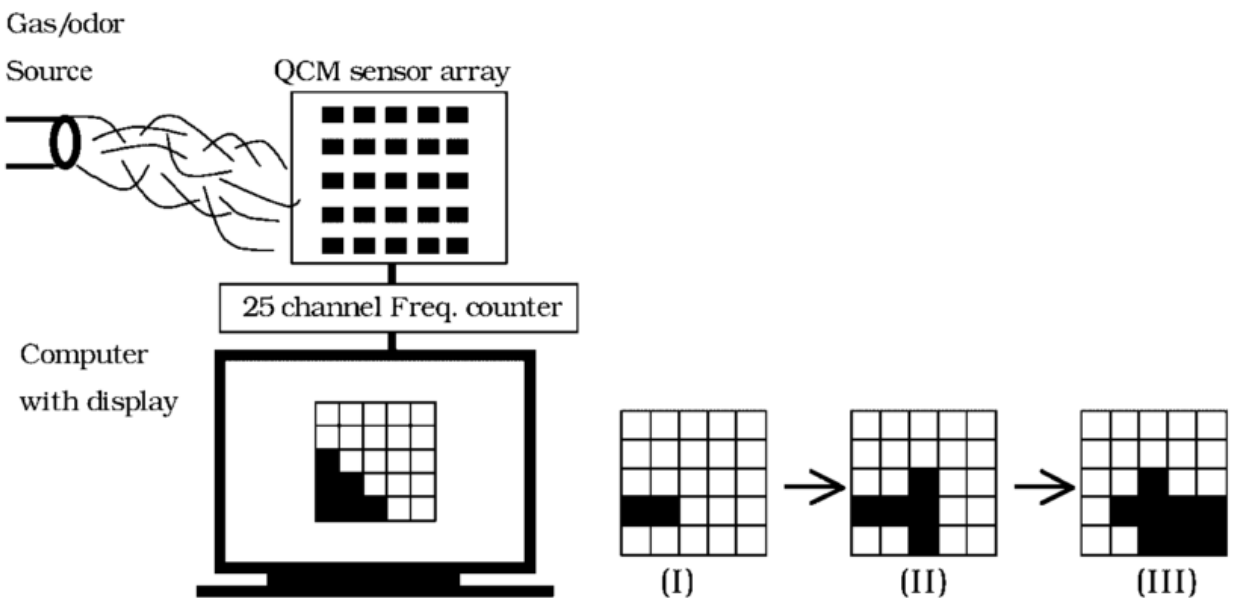
Prof. K. Persaud and the e-nose

Machine olfaction device

By definition: Arrays of broadly-selective chemical sensors combined with a pattern recognition engine

Technologically: A low-cost alternative to instruments of analytical chemistry (or expert panels)

Conceptually: Attempt to mimic the biological olfactory system



[Pearce et al., 2003]

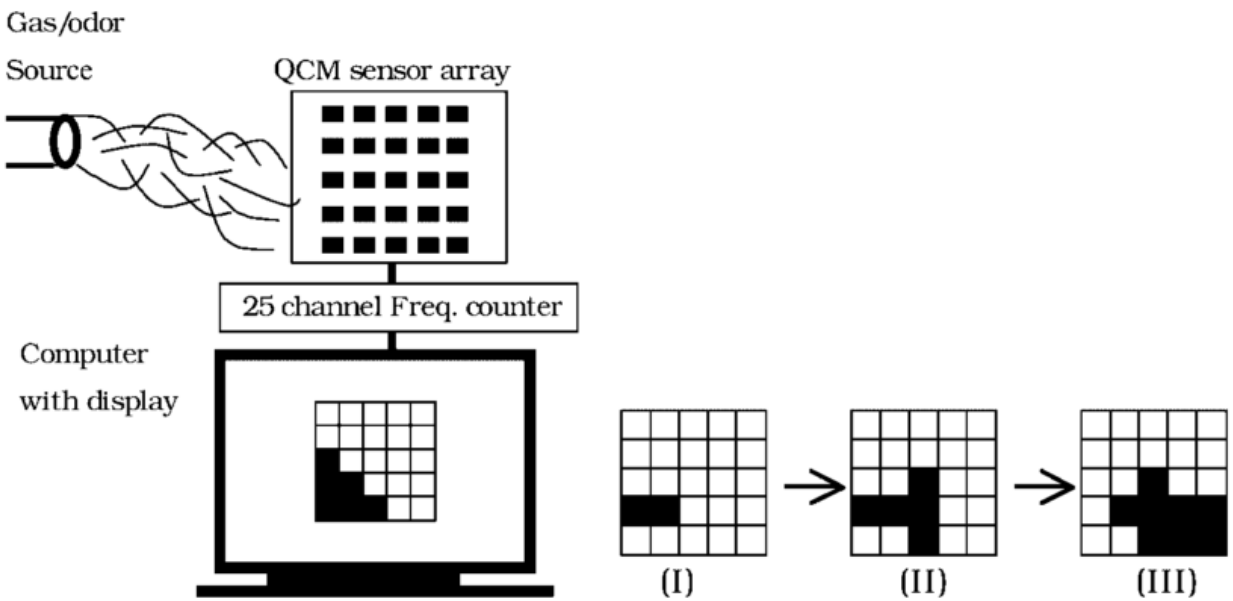
Machine olfaction device

Gas delivery system Prepare and deliver samples to sensors

Array of gas sensors From chemical-physical quantities to signals

Interface electronics Operation and digital-to-analog conversion

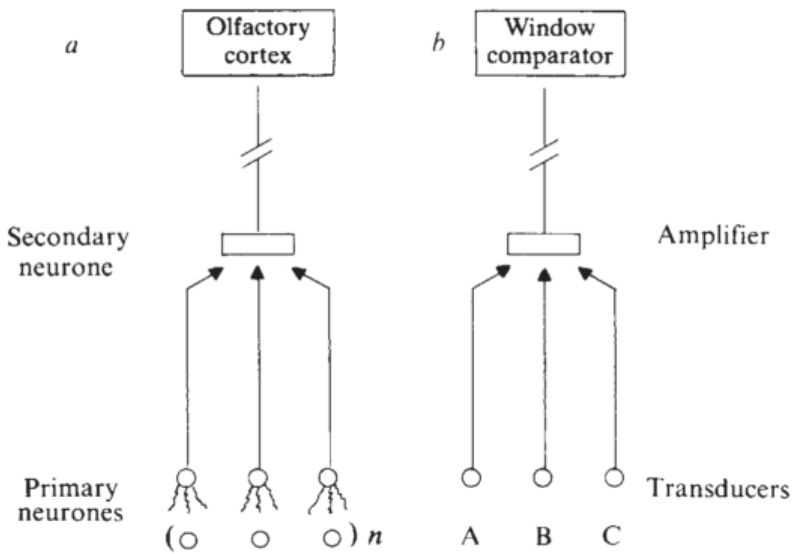
Data processing unit Digital signals to information pieces



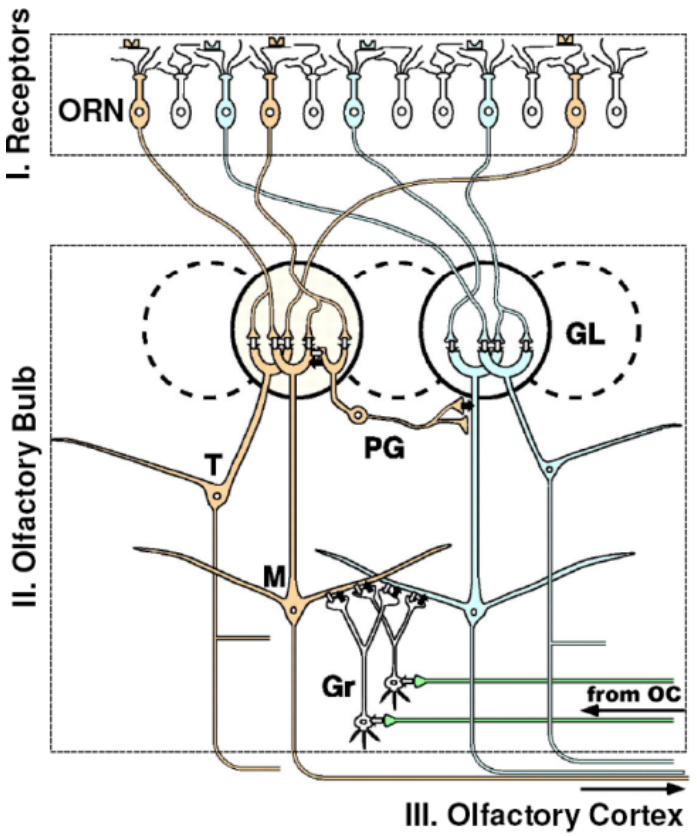
[Pearce et al., 2003]

Findings in biology

[Persaud and Dodd, 1982]



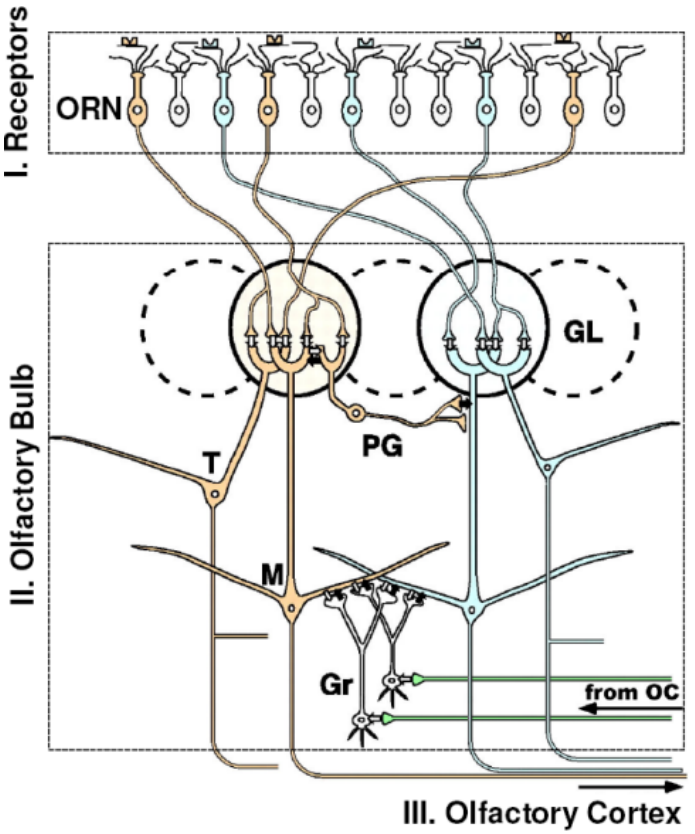
[Mori et al., 1999]



Findings in biology

Early findings

- Seven trans-membrane proteins [Buck and Axel, 1991] (The Nobel Prize)
- Receptors (ORNs) respond to odotopes [Shepherd, 1987], [Shepherd, 1994]
- Ordered convergence to glomeruli (GL) [Vassar et al., 1994]



[Mori et al., 1999]

Bioinspired data processing

First neuromorphic models (in silico)

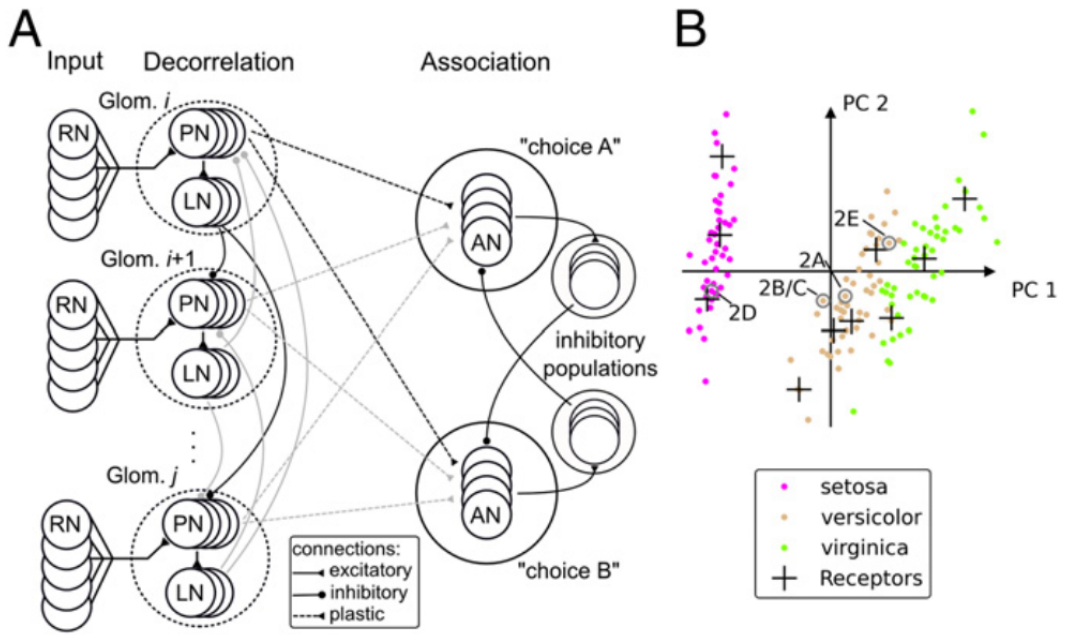
- Convergent architecture for increased sensitivity [Pearce et al., 2001]
- Dimensionality-reduction technique inspired by ORN convergence [Perera et al., 2006]
- Concentration normalization with a model in Olfactory Bulb (OB) [Raman and Gutierrez-Osuna, 2006]
- Increasing separability by Hebbian/anti-Hebbian learning rule [Gutierrez-Galvez and Gutierrez-Osuna, 2006]

First neuromorphic chips

- Implementation of the insect macroglomerular complex in Antenal Lobe (AL) [Pearce et al., 2013]

Neuromorphic classifier on iris data set

- Rapidly converged to a representation
- The correct association established after a few spikes
- Slightly worse performance vs. a naive Bayes classifier
- Especially reliable classification in class-overlapped samples



[Schmuker et al., 2014]

Thesis background

Topics on the focus of this presentation (related to the thesis' contributions)

- Biomimetic robots for machine olfaction
- Drift model
- Data simulations and benchmarks

Topics related to the thesis

- Biological olfaction (Section 1.1.2 in the thesis manuscript)
- Conducting polymer sensors (Section 1.2.1)
- Signal processing (Sections 1.3.1 – 1.3.3)
- Bioinspired signal processing (Section 1.3.5)

Implementation of biomimetic robots

Target

Autonomous robots with embedded computations to resolve real-world scenarios like odor source localization

Open issues

- Low number of gas sensors in arrays
- Neuromorphic computations accomplished remotely
- Design of neuromorphic chips is still a challenge

Existing solutions

- Neural simulator IQR (software tool)
- Mobile robotic platforms with multimodal sensing
- Embedded technology for personal computers (PC)
- Unix-like operating systems (OS)

Drift phenomenon

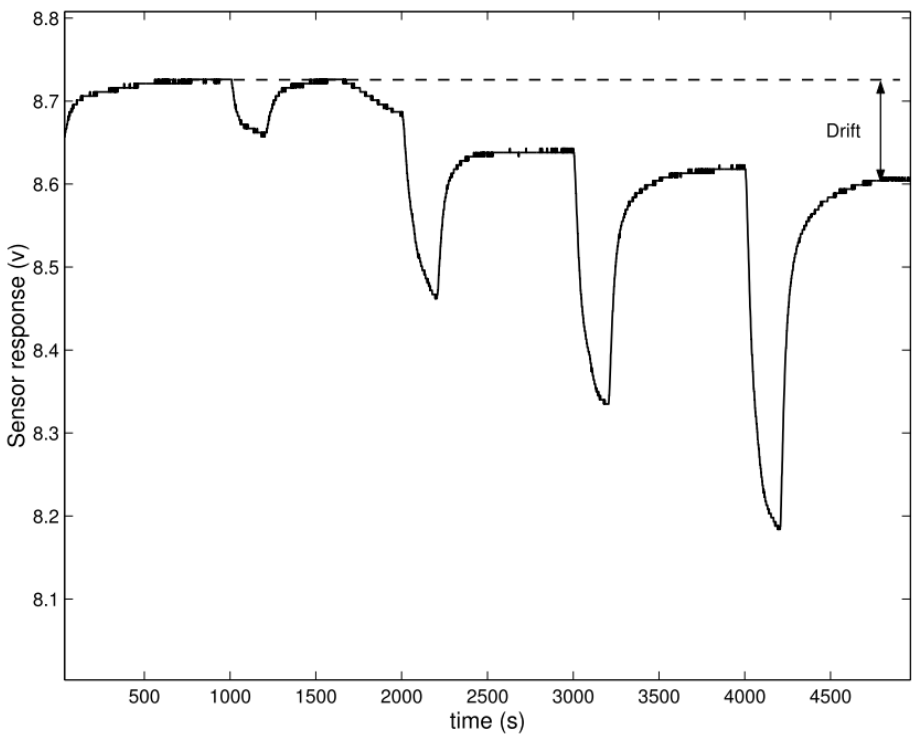
General definition

Gradual changes in a quantitative characteristic that is assumed to be constant over time

Drift in chemosensors

Instrumentation long-term noise (similar to batch effects)

Complex and inevitable effect due to several sources: sampling protocol, environmental conditions, etc.



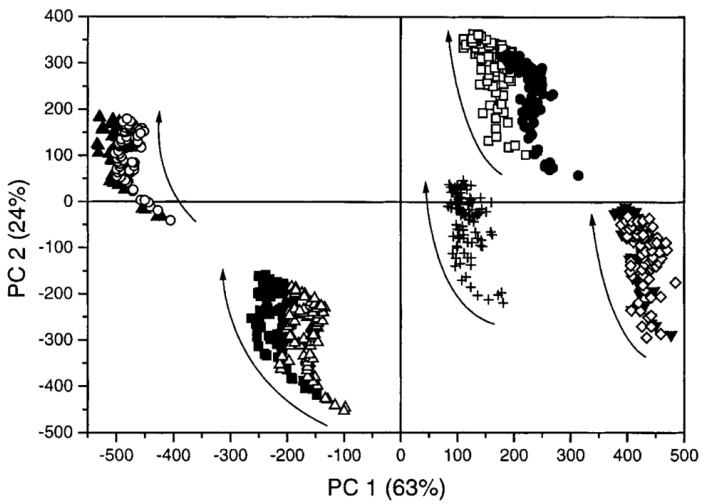
[Bermak et al., 2005]

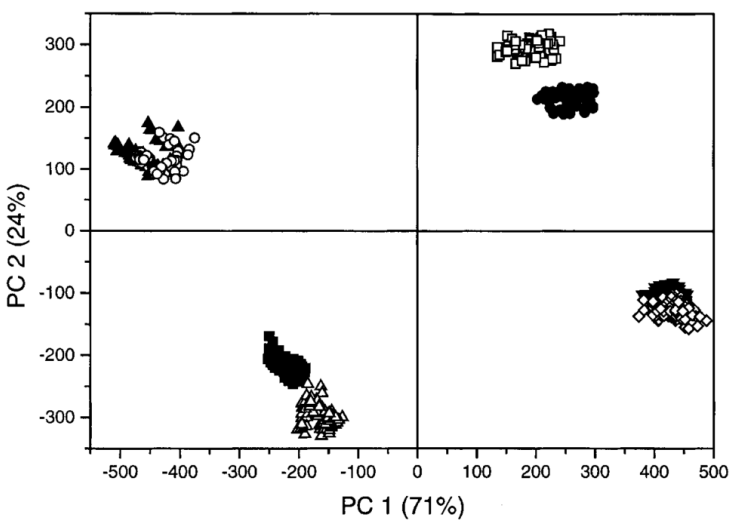
Multivariate correction of drift

A reference method of Component Correction (CC) [Artursson et al., 2000]

- Drift is a subspace $\mathbf{V}$ of variance common to all classes
- $\mathbf{V}$ is estimated by PCA performed on samples from a reference gas
- The drift noise is removed by CC:

$$\mathbf{X}' = \mathbf{X} - (\mathbf{X}\mathbf{V})\mathbf{V}^T$$





[Artursson et al., 2000]

Data availability

Benchmarks

- First time mentioned Ricardo Gutierrez-Osuna in a review [Gutierrez-Osuna, 2002]

Public data sets

- The need for public data was discussed in the ISOEN 2011
- Lab of Ramon Huerta (UCSD, USA) was the first in publishing data sets at The UCI Machine Learning Repository https://archive.ics.uci.edu/ml (4 data sets to date)

Data simulations

- Many sensor models were published, but there is no any data simulation tool available to the comunity

Thesis goals

Robot implementation

UNIMAN data set

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