Towards an Odor Communication System

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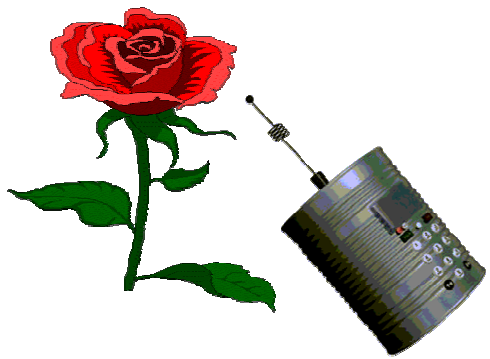
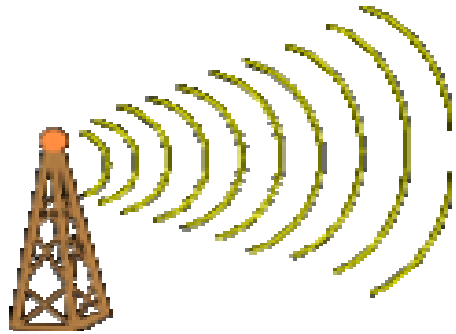
The Weizmann Institute of Science

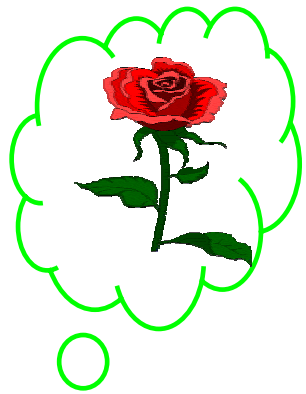
Work done from 1998
initiated by my kid brother, Eli Fisch

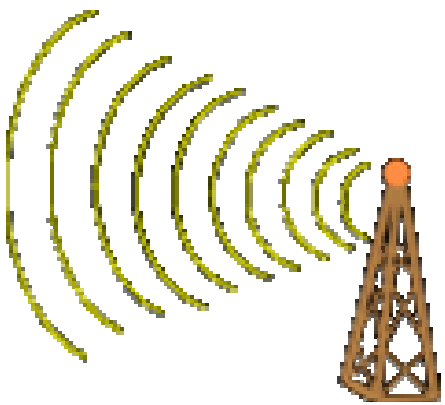
Part 1:
The General Setup

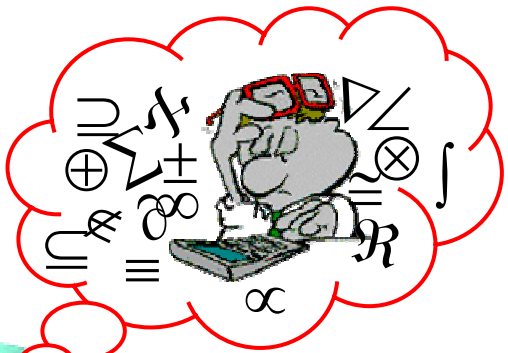
Odor Communication System











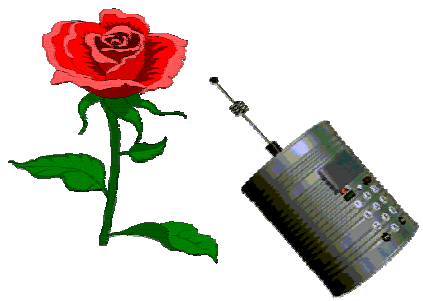
Many exciting & diverse applications

- e-commerce and internet purchasing
- e-games (as part of game strategy too)
- TV and video (e.g., nature programs, movies)
- travel, personal, telephone, e-mail, …
- medical procedures and diagnostics
- odor-related industries

The ultimate dream, & technically the hardest:
Real-time and realistic TV transmission of a cooking program

Hardware: The Sniffer

Maps odor molecules into numbers (e.g., one number per sensor)



$(o;c)$ ⟶ $d^S(o;c)$

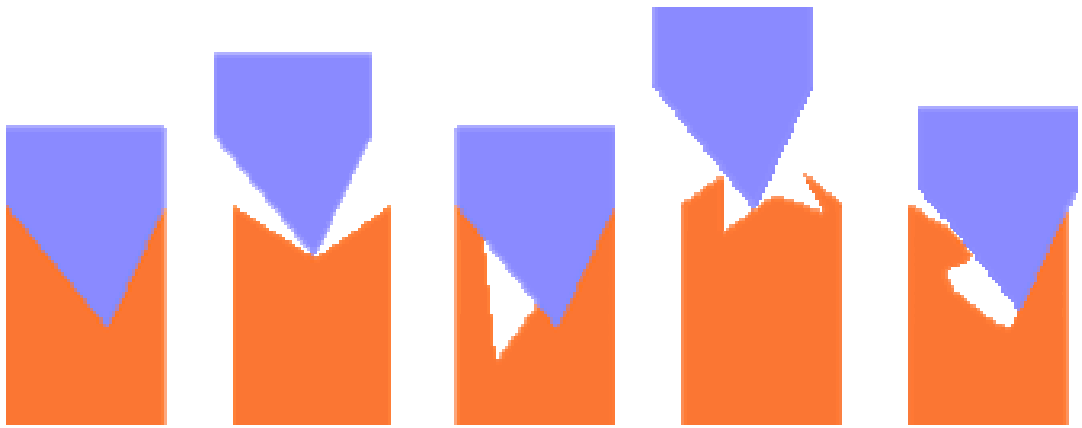
Requirements

- Uniqueness of fingerprint (discrimination)
- Some correlation with odor "quality"
- Small, fast, cheap
- Low complexity of analysis

Expensive eNoses are probably excellent sniffers; but need cheap ones that are good

What is an eNose?

An array of broadly tuned sensors that are different in response



And that's basically how our own noses work too…

eNoses in use

NASA

NCSU

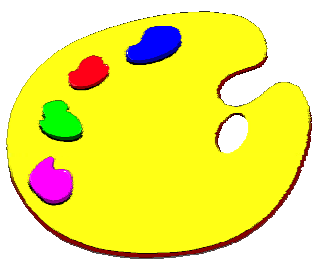
IIT

What they do with these is, by and large, <u>extremely</u> primitive compared to our goal

Hardware: The Whiffer

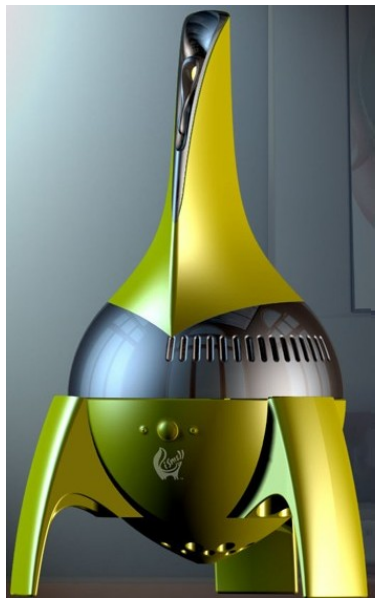
Requirements

- Palette of basic odorants (50-200)
- Precise mixing in specified ratios
- Accurate and timely release


+

= whiffer

Excellent whiffers have been built



iSmell®; built jointly with Eli Fisch, Sagit Fink and others, at Aromix Technologies (later DigiScents Israel)

but commercial venture is on hold for now…

Part 2:
The Algorithmic Scheme

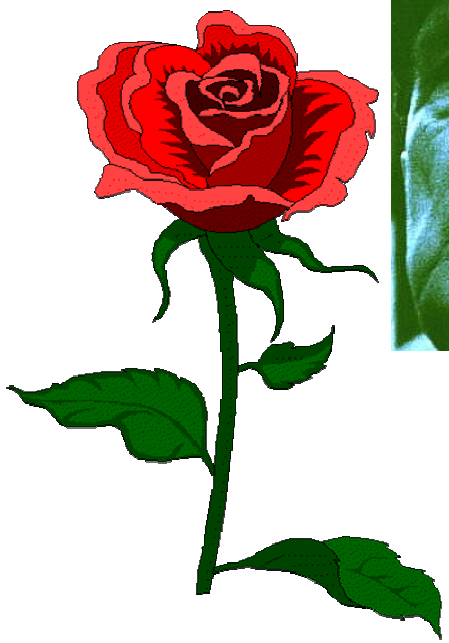
1998
with the help of Doron Lancet

Motivation (Human Olfaction)

We have:

- A non-specific, broadly tuned, "sensor array"
- Exclusive cerebral paths of olfactory neurons
- Qualitatively additive, and reproducible, spatio-temporal patterns
- Limited backtracking (mixing → new odors)
- Olfactory "illusions" (→ can fool the brain)

Unachievable odor space

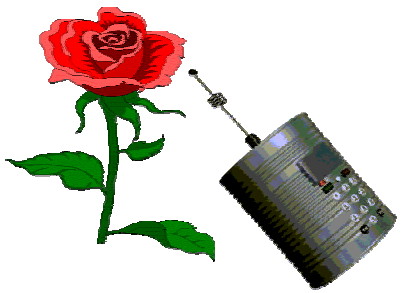


300-500 active receptor types

(o;c) → brain input

Achievable odor spaces

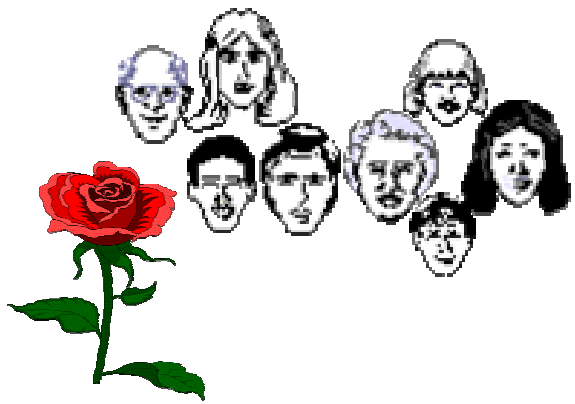
e-nose space



$(o;c) \longrightarrow d^S(o;c)$

m-dimensional

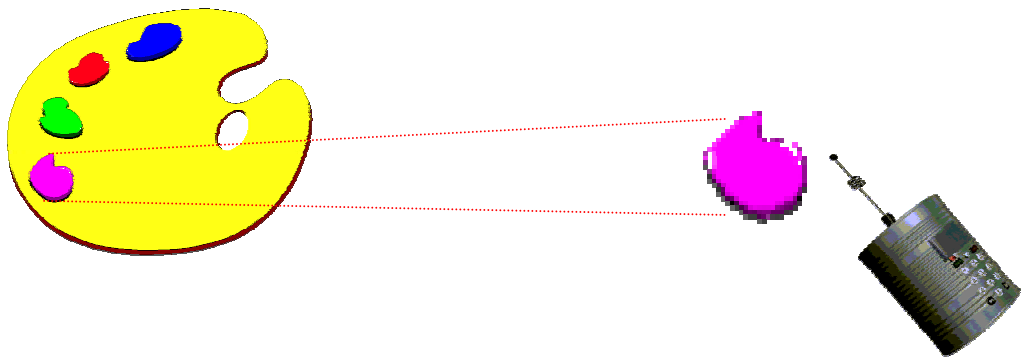
human panel space



$(o;c) \longrightarrow d^H(o;c)$

l-dimensional

Single odorant vector

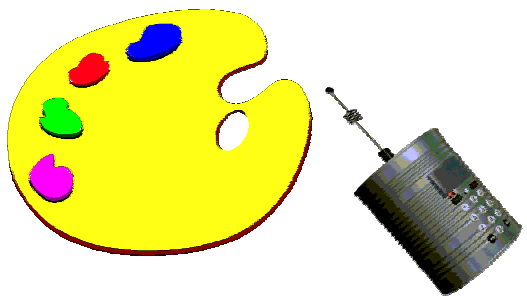


i 'th odorant ⟶ vector p_i

(assuming concentration v_i)

Palette yields matrix

palette of size n

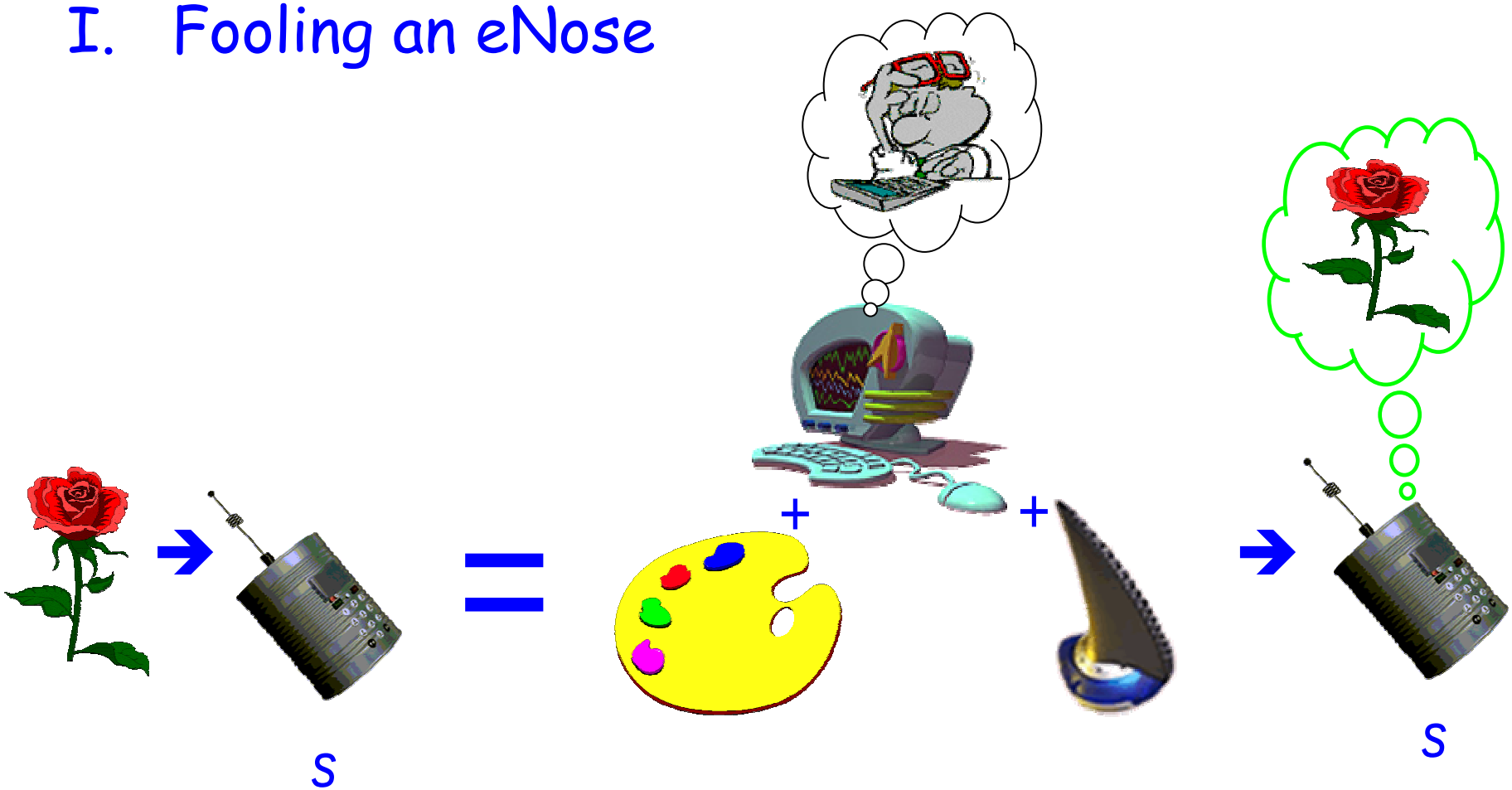


4	2	8	3
1	5	8	5
3	1	2	7
7	7	3	6
2	9	3	5
4	5	1	1
9	3	7	9

palette odorants ⟶ matrix P

The Algorithm (I)

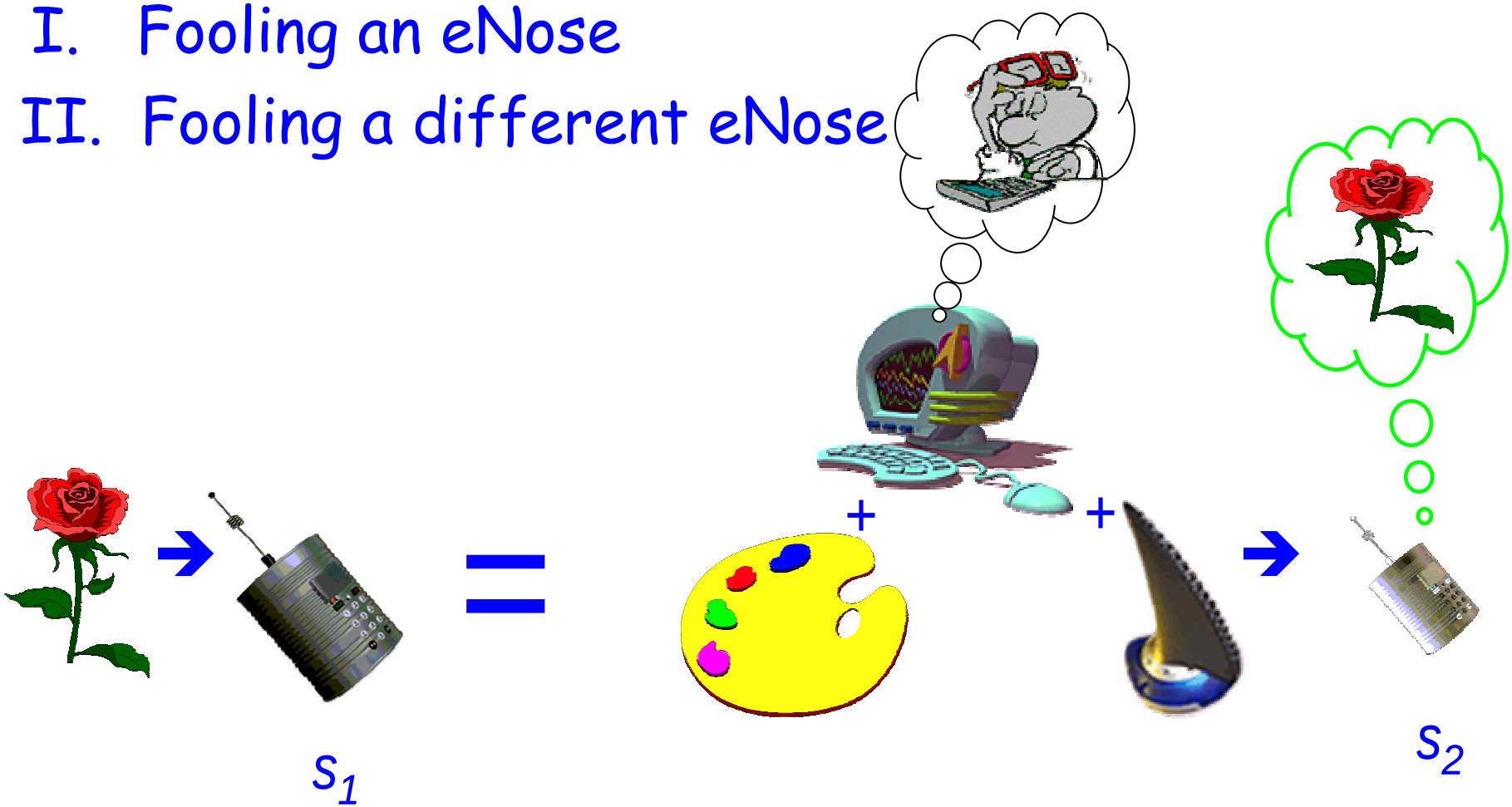
I. Fooling an eNose



The Algorithm (II)

I. Fooling an eNose

II. Fooling a different eNose

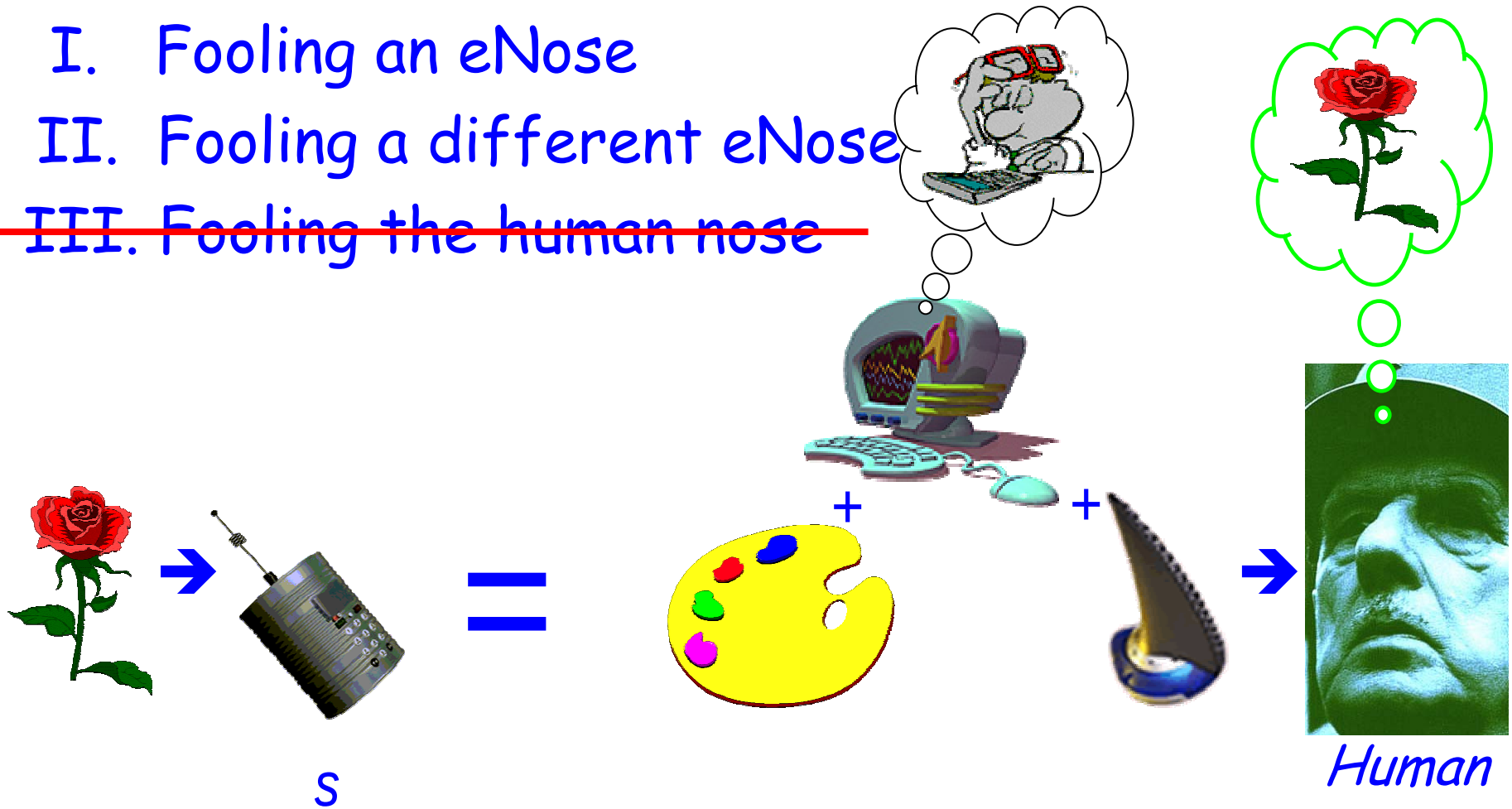


The Algorithm (III)

I. Fooling an eNose

II. Fooling a different eNose

~~III. Fooling the human nose~~



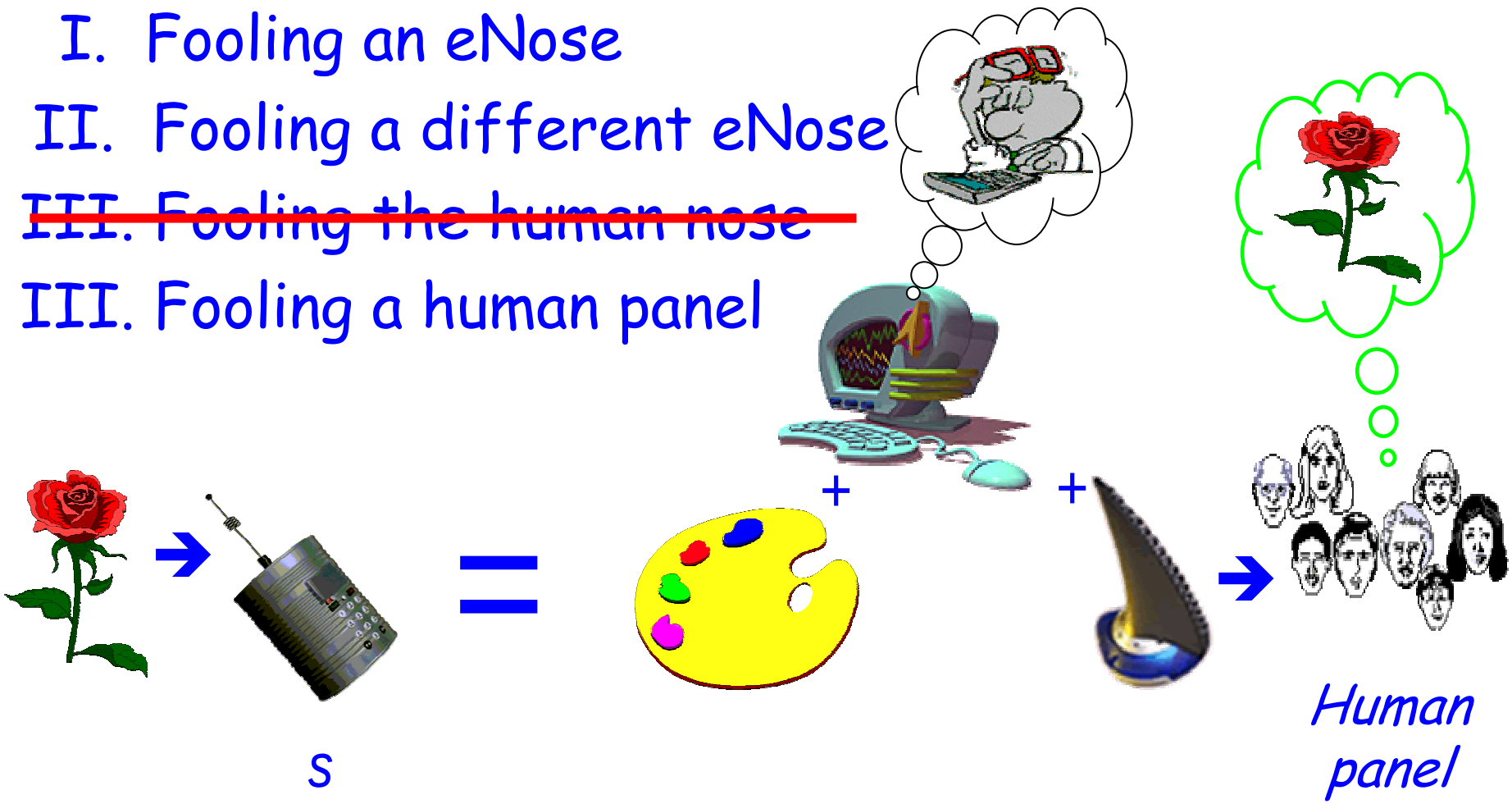
The Algorithm (III)

I. Fooling an eNose

II. Fooling a different eNose

~~III. Fooling the human nose~~

III. Fooling a human panel



S

Assume linear sniffer S

- Concentration linearity

$$d_j^S(o;c) = \alpha_j(o)\cdot c \qquad j = 1, \ldots, m$$

- Mixing linearity

$$(o_1;c_1),\ (o_2;c_2),\ \ldots,\ (o_n;c_n)$$

$$d_j^S = \alpha_j(o_1)c_1 + \alpha_j(o_2)c_2 + \ldots + \alpha_j(o_n)c_n$$

$$j = 1, \ldots, m$$

For palette P and vector of concentrations v, $P \cdot v$ is an odor signature in S-space.

Hence, given an odorant $(o;c)$, the following least squares problem captures mimicking o with P :

find v so as to minimize

$$\left| P \cdot v - d^S(o;c) \right|$$

I. Fooling an eNose

1. Use S to digitize odorant $(o;c)$; yields $d^S(o;c)$

2. Given palette P analyzed using S,
   find v so as to minimize $|P \cdot v - d^S(o;c)|$

II. Fooling a different eNose

1. Use S_1 to digitize odorant $(o;c)$; yields $d^{S_1}(o;c)$

2. Transform $d^{S_1}(o;c) \rightarrow d^{S_2}(o;c)$

3. Given palette P analyzed using S_2,
   find v so as to minimize $\left| P \cdot v - d^{S_2}(o;c) \right|$

We have to find a general mapping from $d^{S1}(o;c)$ to $d^{S2}(o;c)$

- different dimensionality
- different sensors
- different response patterns

How can we find this mapping?

- Artificial neural networks
- Genetic algorithms
- Polynomial fitting
- Direct analysis of the sensors' signals
- And more …

III. Fooling a human panel

1. Use S to digitize odorant $(o;c)$; yields $d^S(o;c)$

2. Transform $d^S(o;c) \rightarrow d^H(o;c)$

3. Given palette P analyzed using H,
   find v so as to minimize $\left| P \cdot v - d^H(o;c) \right|$

The mapping

We have to find a general mapping from $d^S(o;c)$ to $d^H(o;c)$

In principle, can use methods like those used to find the mapping between two different eNoses

But,… this could be more complicated, since the spaces are very different

Yet,… there is encouraging evidence; e.g., Nestle used eNose to predict human panel results on off-odors in packaging materials

Working with a human panel

Psychophysical work; best to use comparative, rather than absolute, questioning techniques

Must build up lots of information on $d^H(o;c)$

Must "pass the palette through" *H*

Involves much careful and consistent work; using a wide spectrum of odors

Is our brain linear?

- Concentration linearity?

  Stevens' law: $I = kc^r$

  For small enough regions of concentration, we can assume the linear approximation $I = k'c$

- Mixing linearity?

  Several results (incl. olfactory bulb response patterns) indicate: probably yes, in many cases

Part 3:
Work in Progress

1999-2003
mostly joint with PhD student Liran Carmel

MosesII: desktop eNose ($70K)

Modular Sensor System;
II'nd generation

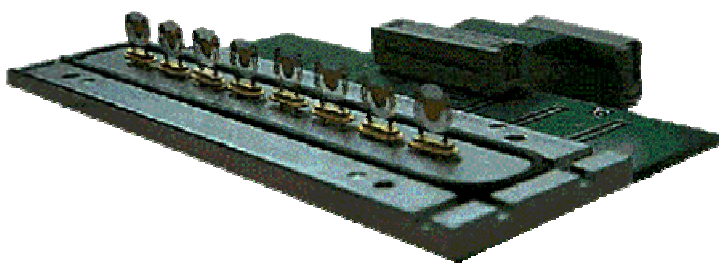
headspace auto-sampler

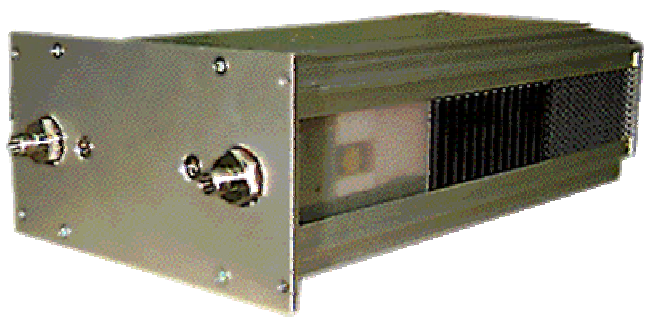
personal computer

- sixteen sensors (2 x 8)
- three input channels
- temperature & humidity sensors
- flow sensor & controller
- pump

8 Quartz MicroBalance sensors (QMB)

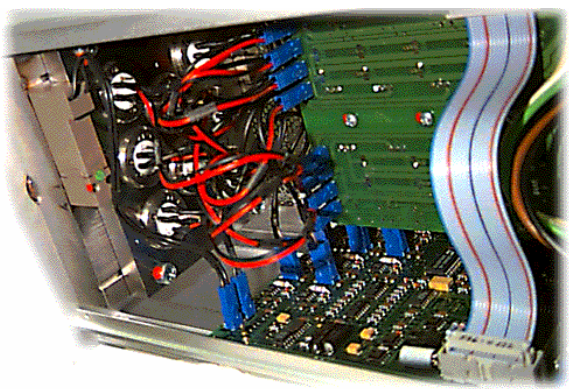
- piezoelectric quartz crystal
- polymer coating
- acoustic waves
- frequency counter

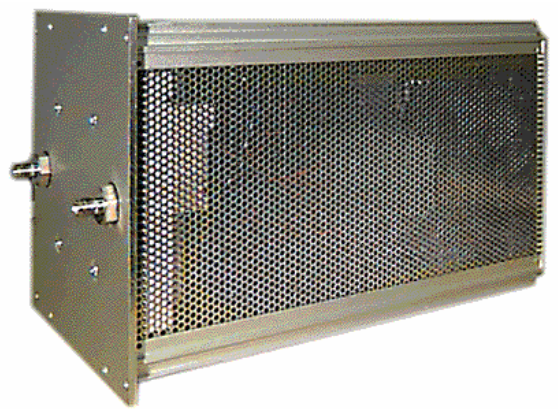




8 Metal Oxide Sensors (MOS)

- metal oxide
- catalytic additives (doping)
- heater coil
- surface combustion reactions





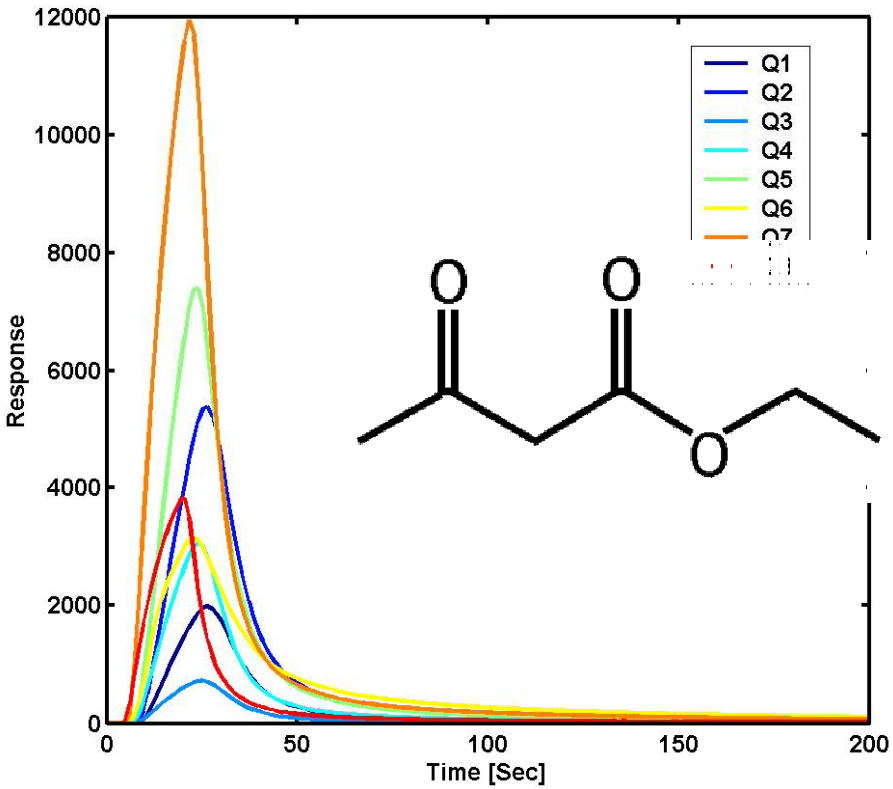
Cyranose320: handheld eNose ($7K)

(have recently begun work on this)

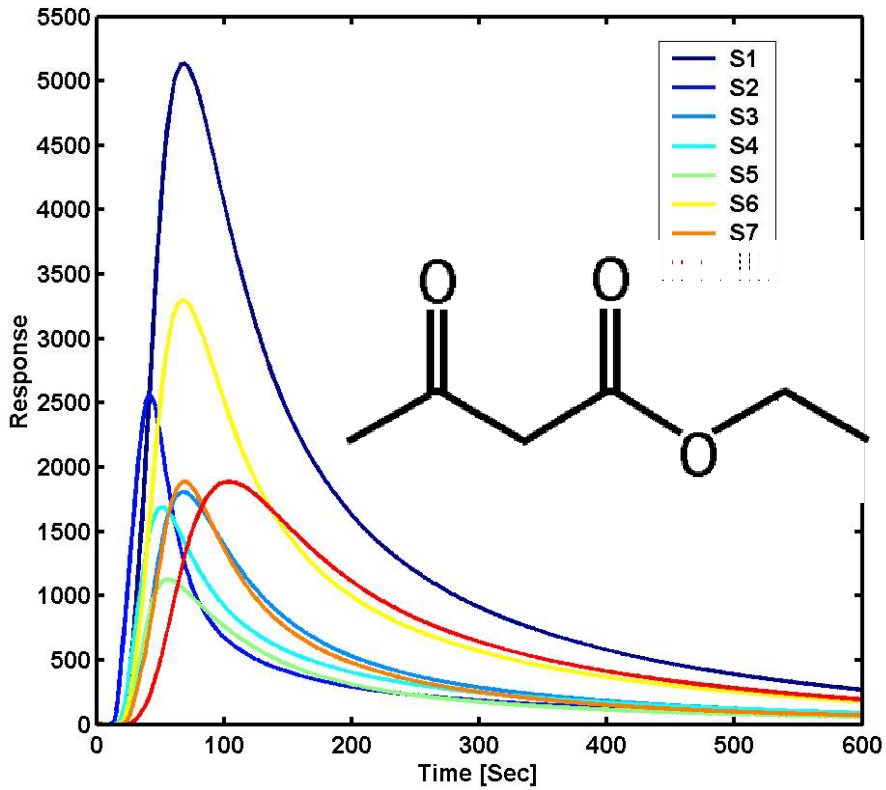
32 different conducting polymer sensors

Example (MosesII): butyl butyrate

QMB



MOS



So, what have we been doing?

- Mathematical modeling of response
- Odor identification
- Identification w/ concentrations
- Analysis of mixing
- Mappings between eNoses
- (A little human panel work)

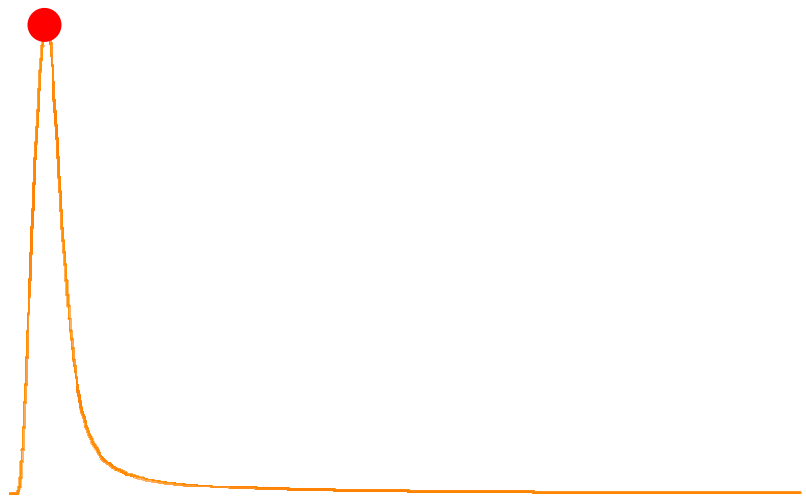
Mathematically modeling the response

By feature extraction and shape modeling

An attempt to match chemistry
with workable mathematics

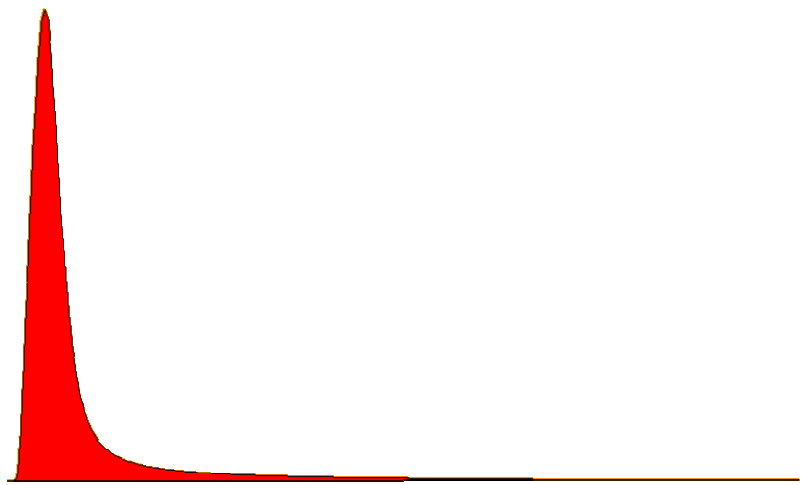
Plausible feature 1

- peak



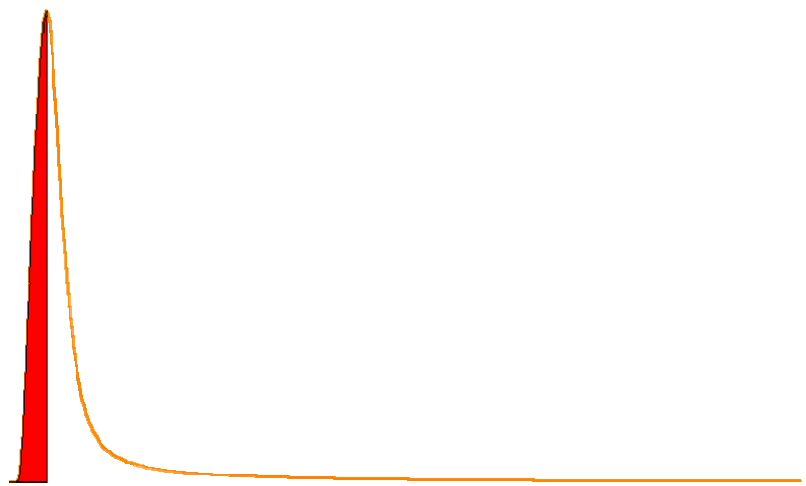
Plausible feature 2

- peak
- area



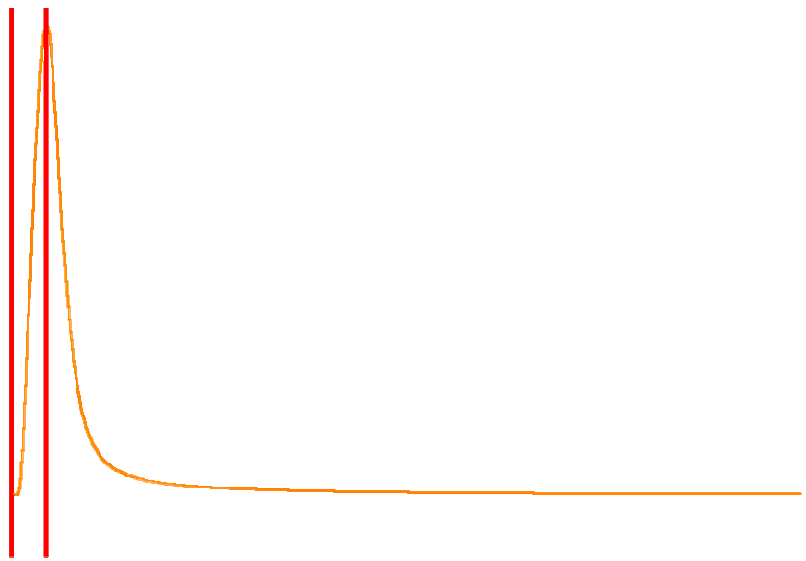
Plausible feature 3

- peak
- area
- area to peak



Plausible feature 4

- peak
- area
- area to peak
- time to peak



Our Lorentzian Shape Model

Resulted from playing with the application of some simple physical principles to the measuring system

$$R(t) = \begin{cases} 0 & t < t_i \\ \beta\tau \tan^{-1}\left(\dfrac{t - t_i}{\tau}\right) & t_i \le t \le t_i + T \\ \beta\tau\left[\tan^{-1}\left(\dfrac{t - t_i}{\tau}\right) - \tan^{-1}\left(\dfrac{t - t_i - T}{\tau}\right)\right] & t > t_i + T \end{cases}$$

β amplitude

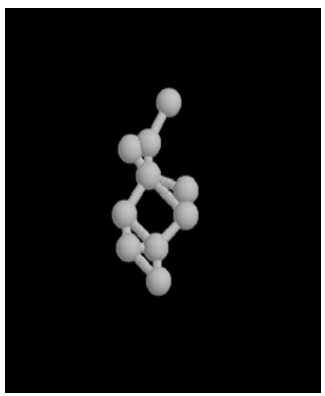
t_i rise time

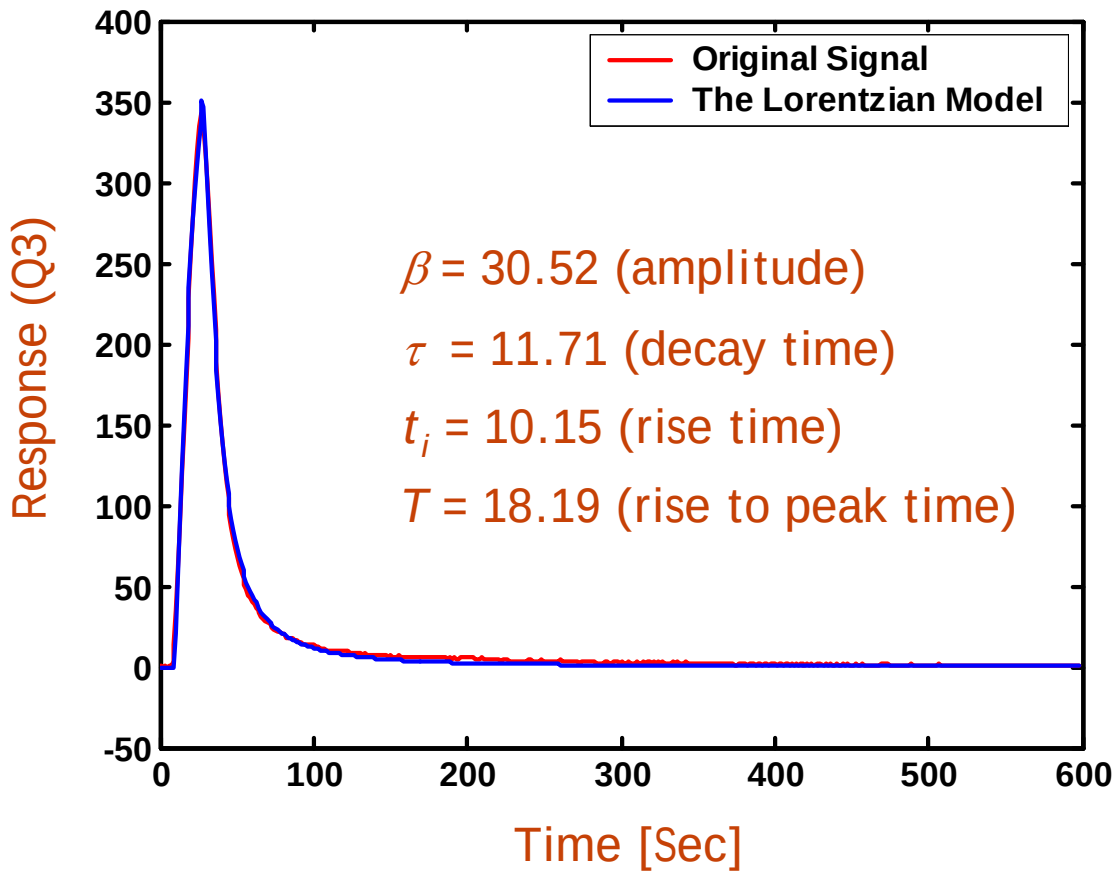
τ decay time

T rise to peak time

Example

(-)-limonene





What is a shape model good for?

- algorithmic & mathematical workability
- error correction
- compression, calibration, drift, etc.
- efficient outlier detection
- high classification rate

Odor identification

Classify an incoming unknown sample

Used database of 70 pure chemicals

- Very different in nature ⇨ different scaling
- But uniform working conditions

Chemicals used

1s-(-)-beta-pinene
butyl butyrate
citral
ethyl acetoacetate
isoamyl formate
terpinolene
3,4-hexanodione
anethole supra
carvacrol
d-carvone
Dihydrocarvone
terpinotene
vanillin iso-butyrate
1s-(-)-alpha-pinene
R-(-)-limonene
S-(-)-limonene
1-methylpyrrole
2-acetylpyridine
cis-3-hexenyl acetate
ethyl isobutyrate
ethyl isovalerate
2-methyl-4-propyl-1,3-oxathiane
Dihydronootkatone
Carveol
dihydrocarvyl
ethyl-2-methyl-4-pentenoate
phenylacetaldehyde dimethyl acetal
phenylacetaldehyde diisobutylacetal
2,3-heptanedione
2-methyl-2-pentenal
acetyl propionyl
acetylbutyryl
1-phenyl-1,2-propanedione
2,3-hexanedione
4-methylanisole
acetal

Chemicals used (cont.)

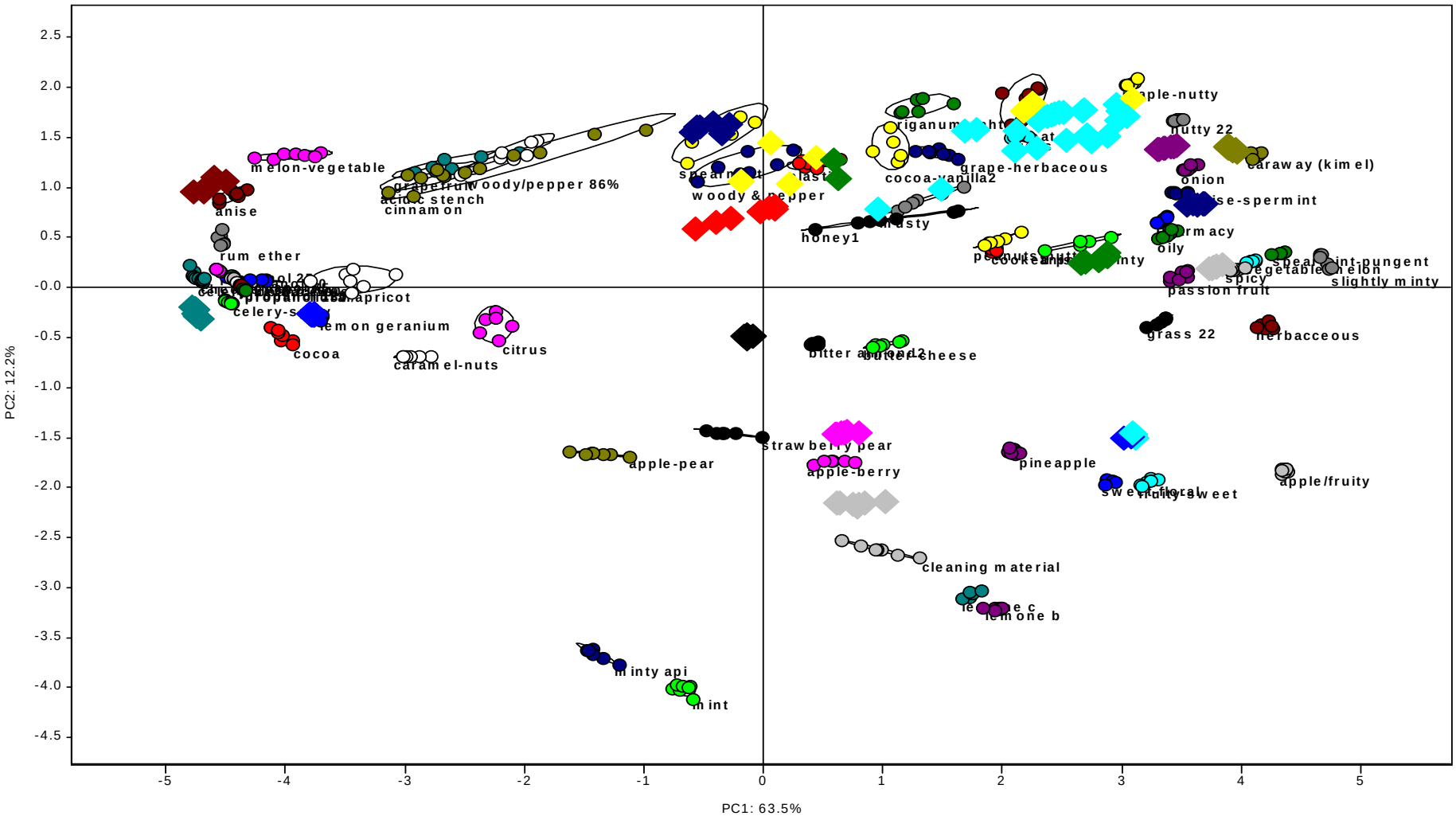
ethylpyrazine
propylidene phthalide
amyl butyrate
butyl butyryl lactate
dihydrocarveol
ethyl valerate
trans-2-methyl-2-pentenal
valencene
carvacryl ethyl ether
ethyl-3-methylthiopropionate
geranyl-2-methyl butanoate
L-carvyl propionate

nootkatone ex valencene 86%
tetrahydrocarvone
butylidene phthalide
dihydroanethole
methyl-2-methylbutyrate
rum ether
trans-2-hexenal
trans-2-hexenol
trans-cinnamaldehyde
cis-6-nonenol
4-methyl-5-thiazolylethyl acetate

alpha-angelica lactone
carvacryl methyl ether
cis-6-nonenal
geranyl undecylenate
4-methyl-5-vinylthiazole
ethyl caproate
ethyl-2-methylbutyrate
ethyl-3-hydroxybutyrate
trans-2-methyl-2-pentenoic
trans-2-octenal
ethyl n-valerate

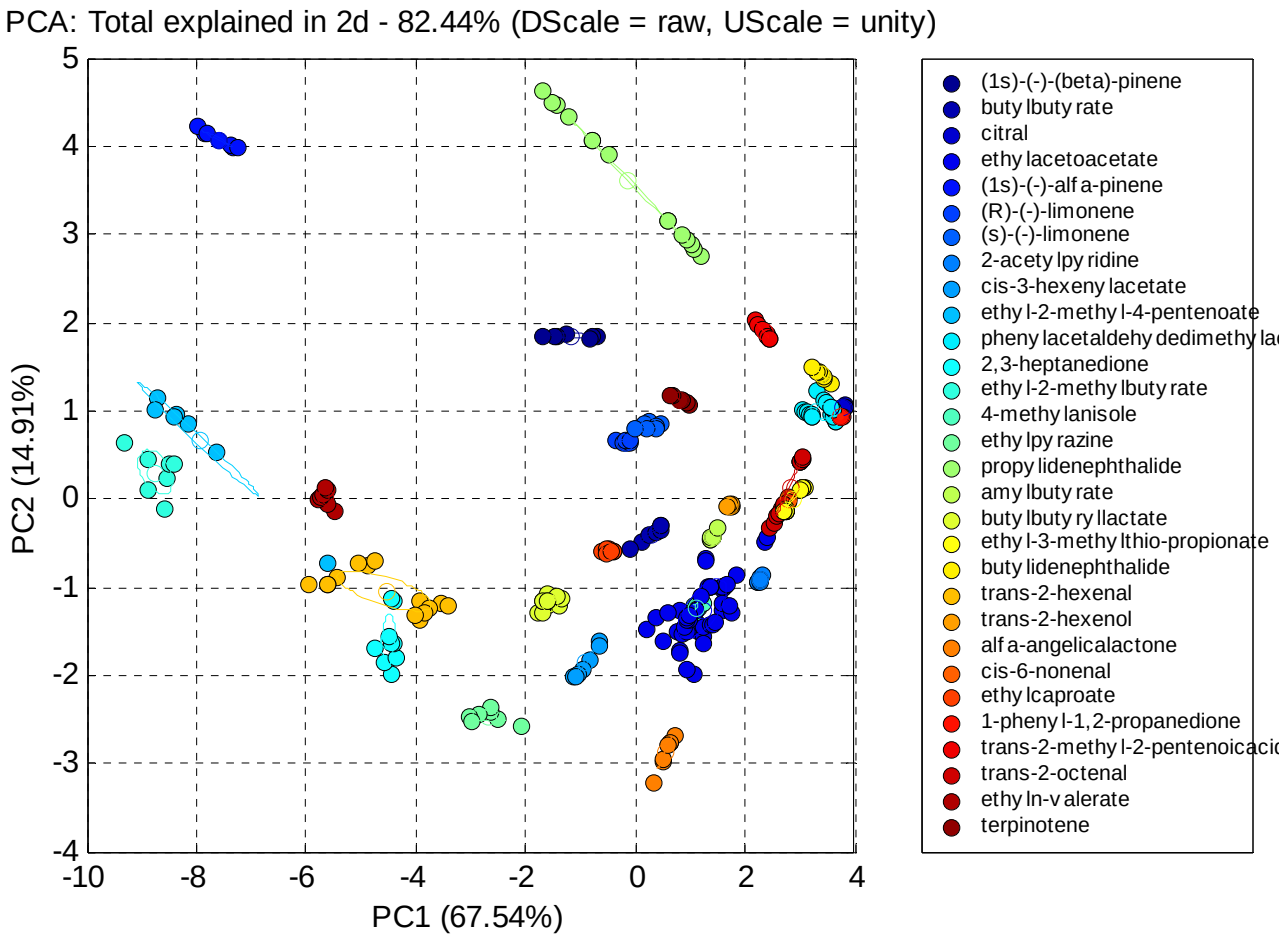
Example – 50 pure chemicals

(2-dim PCA)



Example – 30 chemicals

2-dim principle components analysis (PCA)



Classification algorithms

- K-Nearest Neighbors (KNN)
- Closest group by Mahalanobis distance
- Bayesian classification:
  Linear Discriminant Analysis (LDA)
- Bayesian classification:
  Quadratic Discriminant Analysis (QDA)

Classification results

Success % for 30 chemicals

reference vs. sample: method, ratio

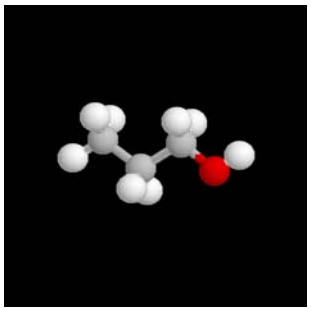
	excess 7:3	random 2:1	random 1:1
KNN	72%	93%	14%
Mahalanobis	22%	92%	4%
LDA	100%	100%	100%
QDA	100%	100%	100%

Identification with concentration

Classify an incoming unknown sample
and determine its concentration

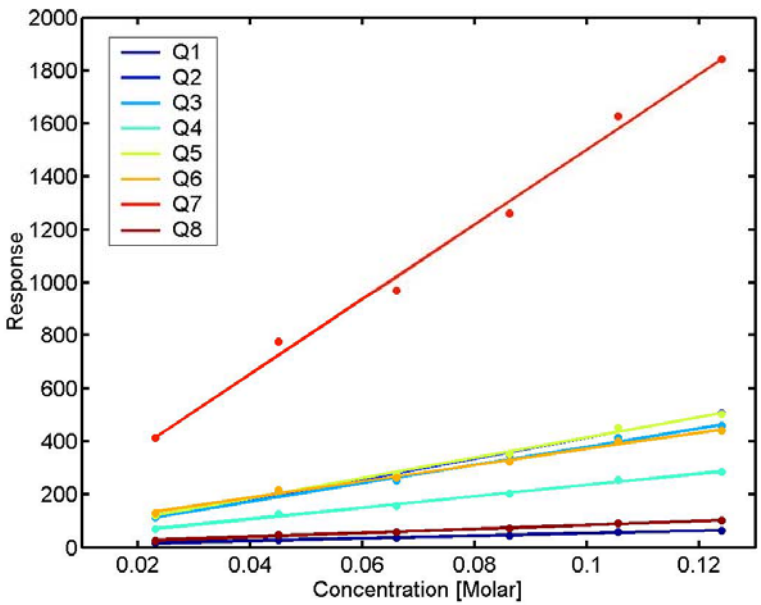
The problem:
It is possible that (o,c) will "fall" on the
same spot as (o',c')

Concentration linearity

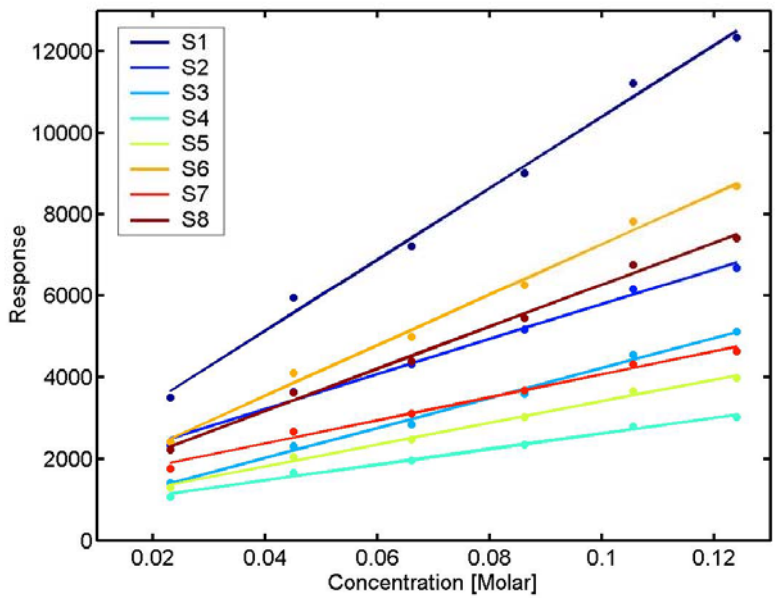


propanol

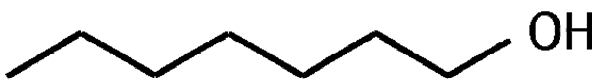
QMB



MOS

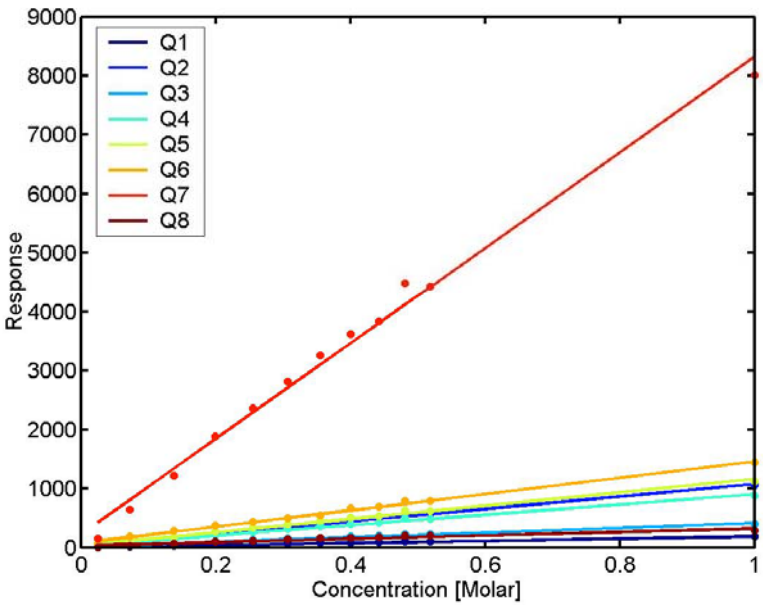


Concentration linearity

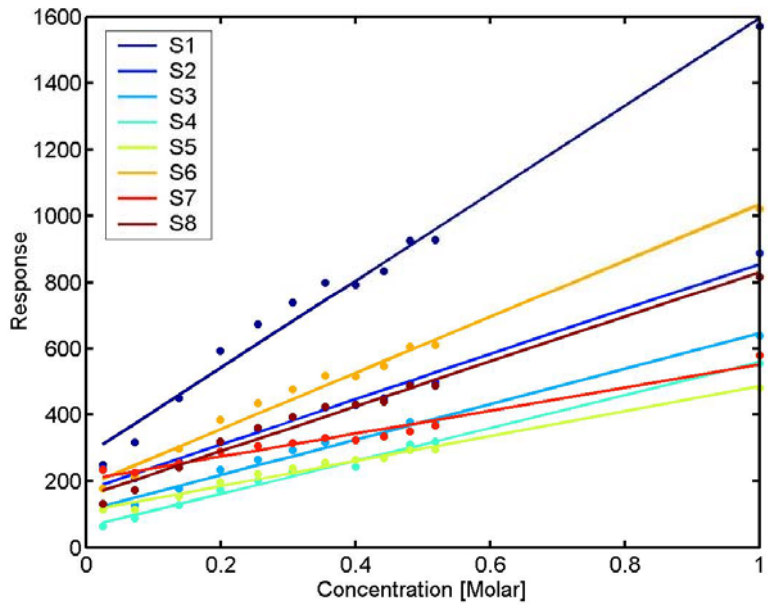


heptyl alcohol

QMB



MOS

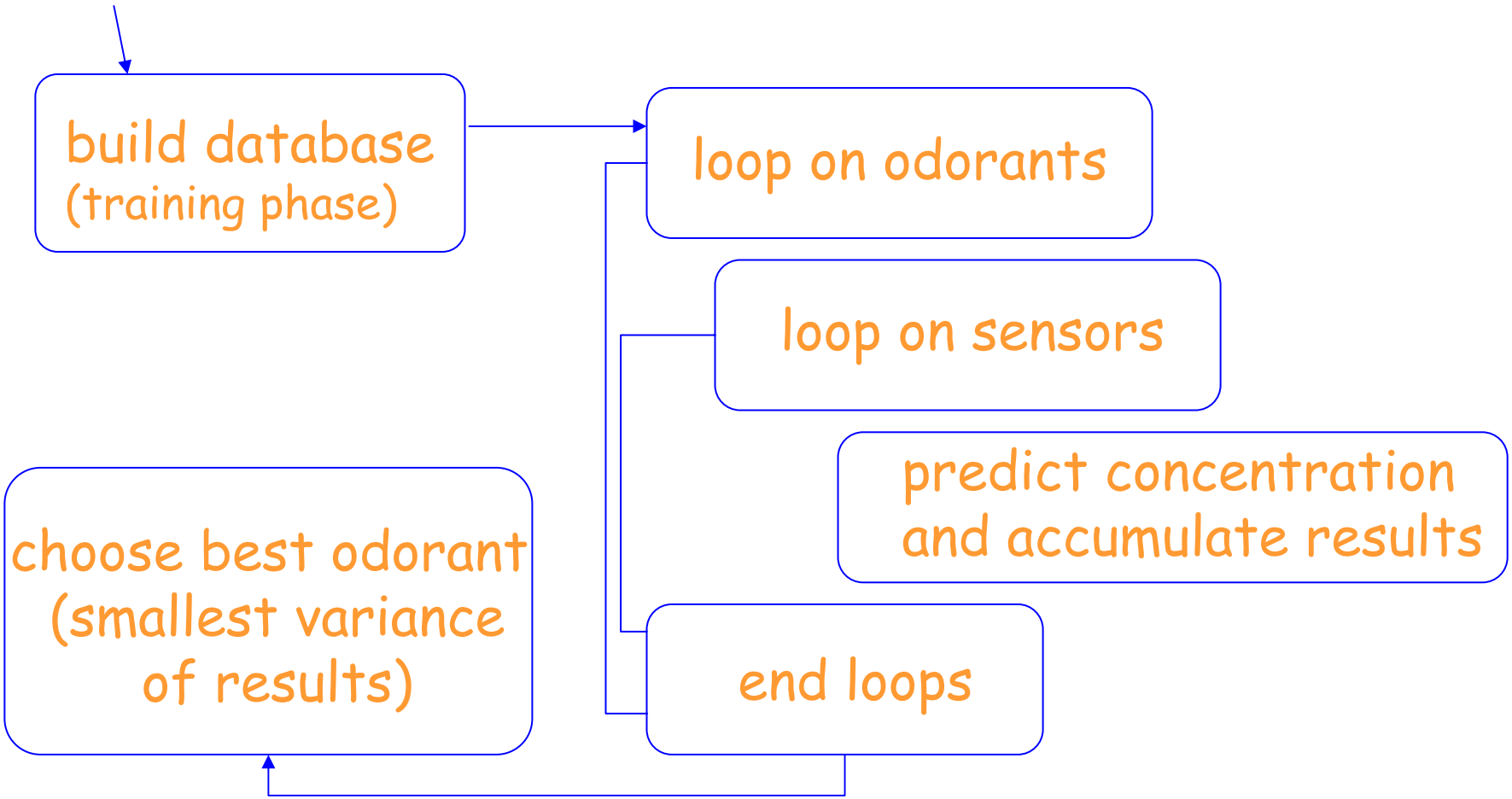


The algorithm

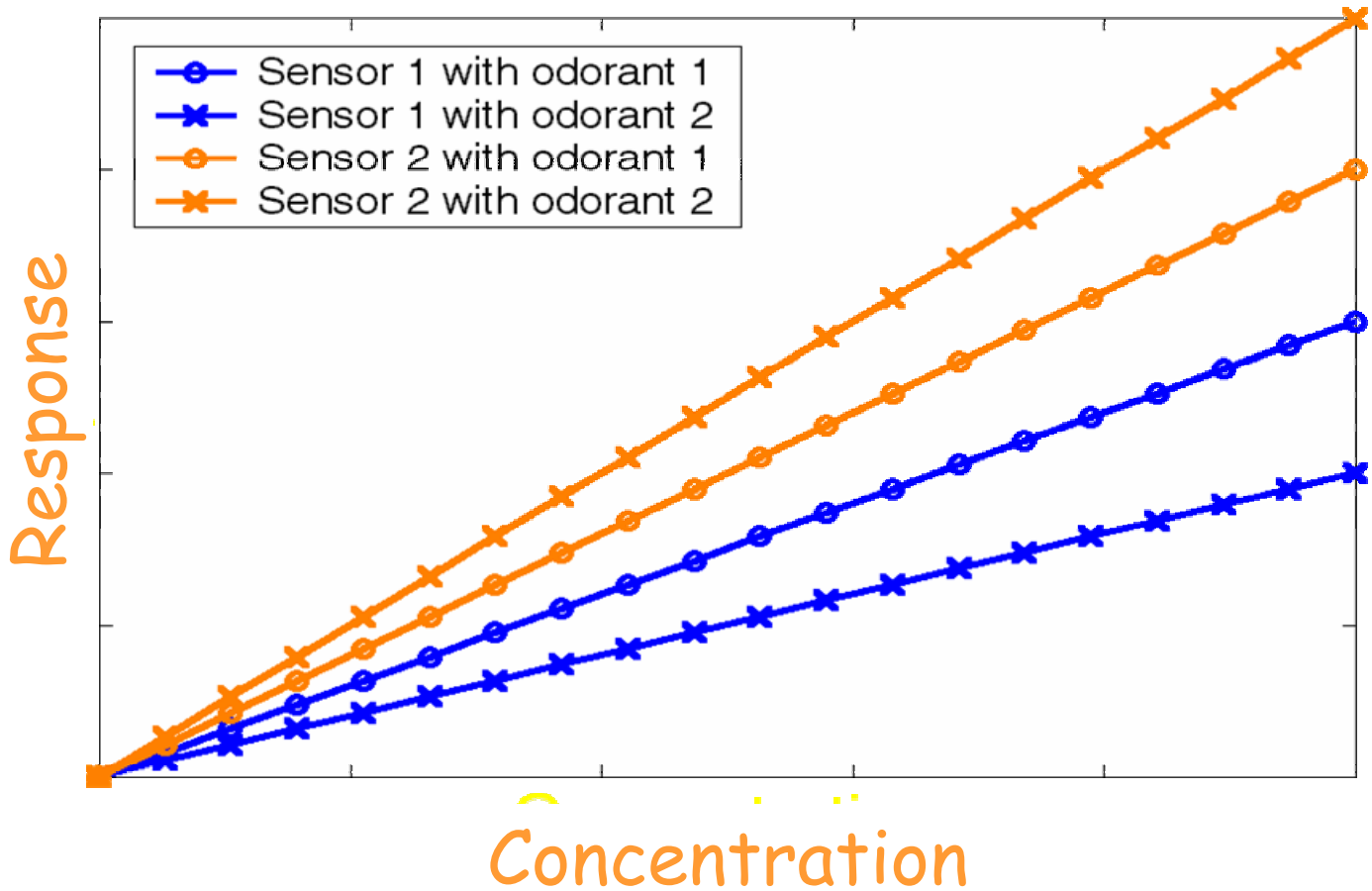
Inspired by J. J. Hopfield, "Odor Space and Olfactory Processing: Collective Algorithms and Neural Implementation", PNAS **96** (1999) 12506-12511

- straightforward and intuitive
- easy to implement
- explicitly using the multiplicity of sensors
- proposed similar ideas for the biological olfactory processing mechanism

Algorithm for identification with concentration

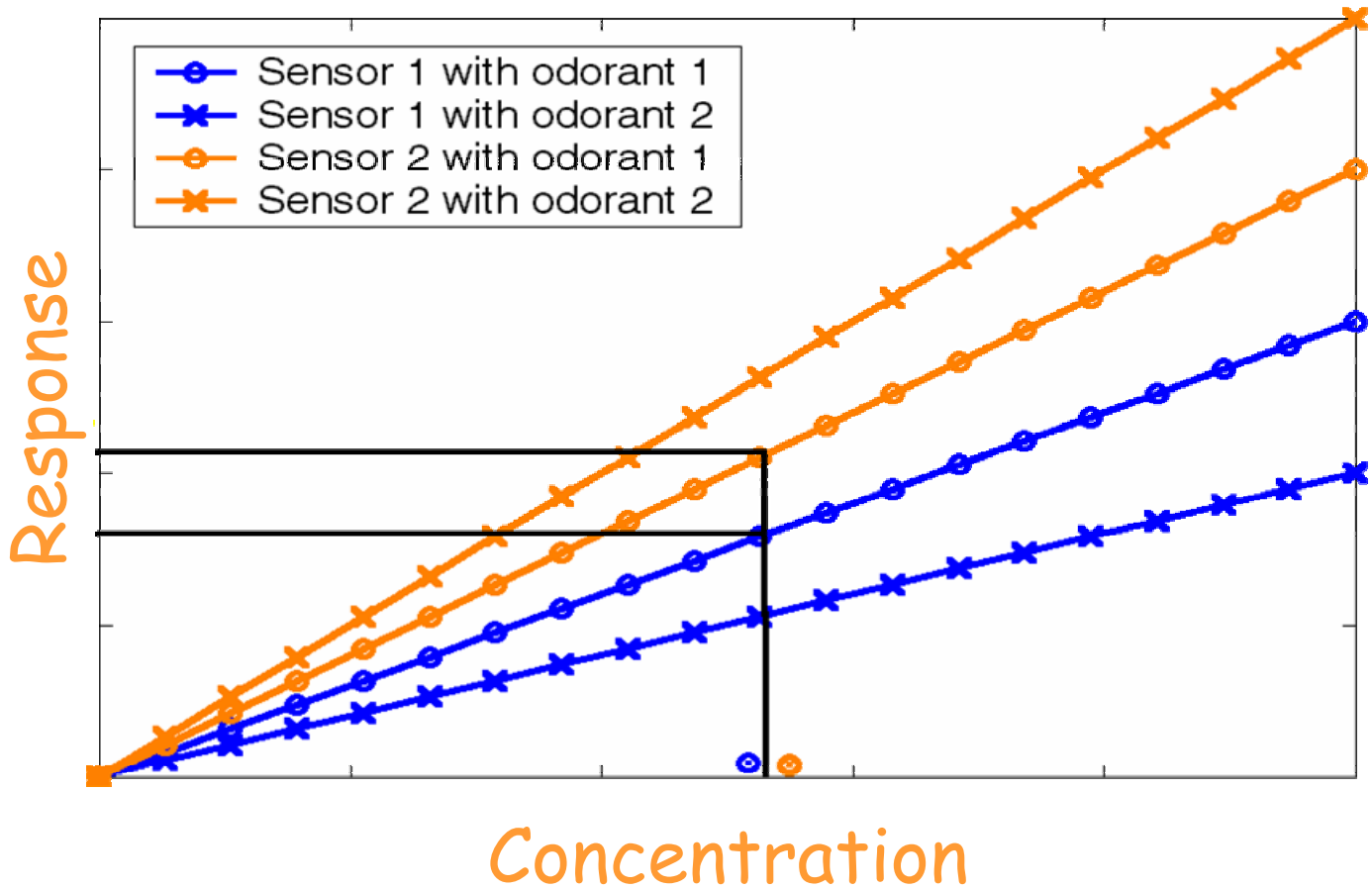


Demonstration



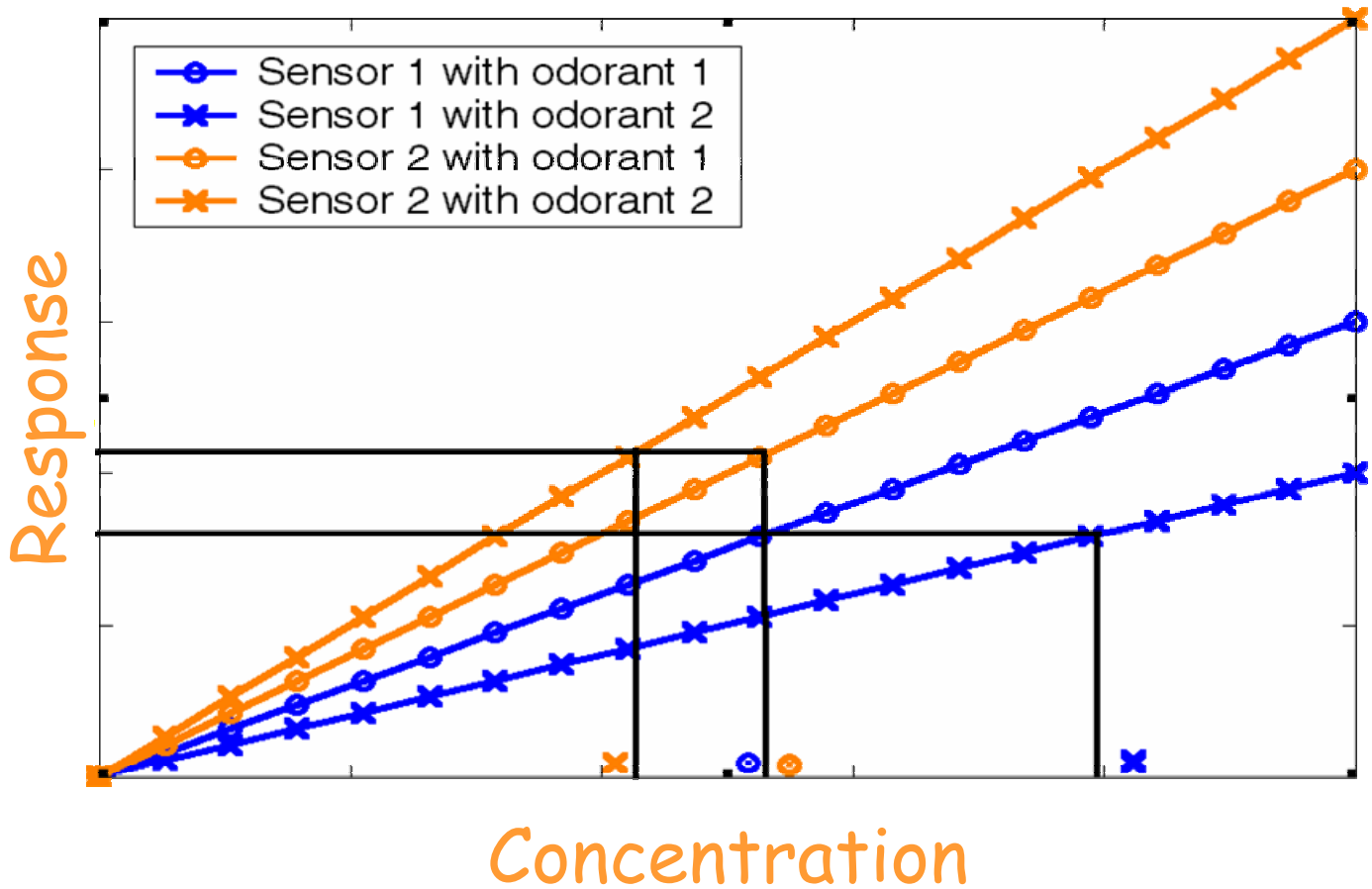
Demonstration

Is it the circle odorant?

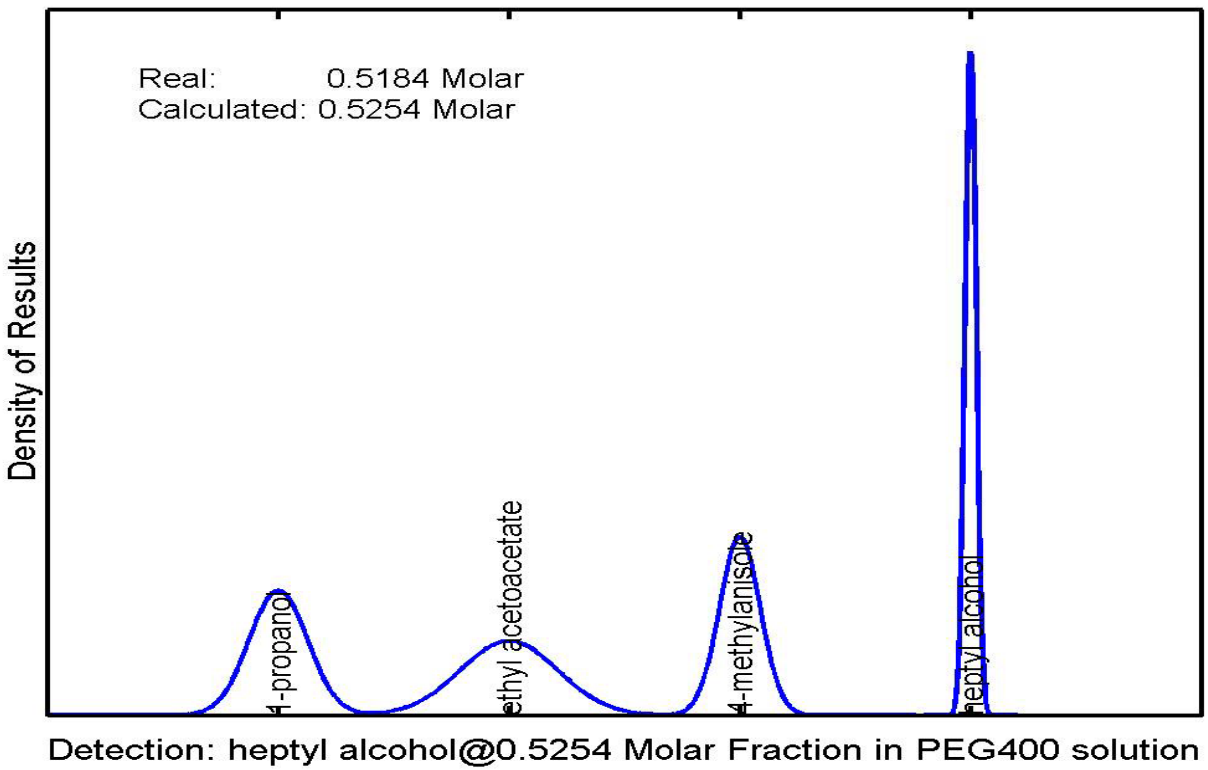


Demonstration

Is it the cross odorant?



Example (identifying w/ concentration)



Results

Applying the algorithm to the training dataset:

100% correct classification

1.4% relative error in concentration prediction

Groups in validation dataset

Group I: candidates at concentrations from within those that were used during the training phase

Group II: candidates at concentrations not present during the training phase

Group III: non-candidates

Mixing odors (⇨ fooling)

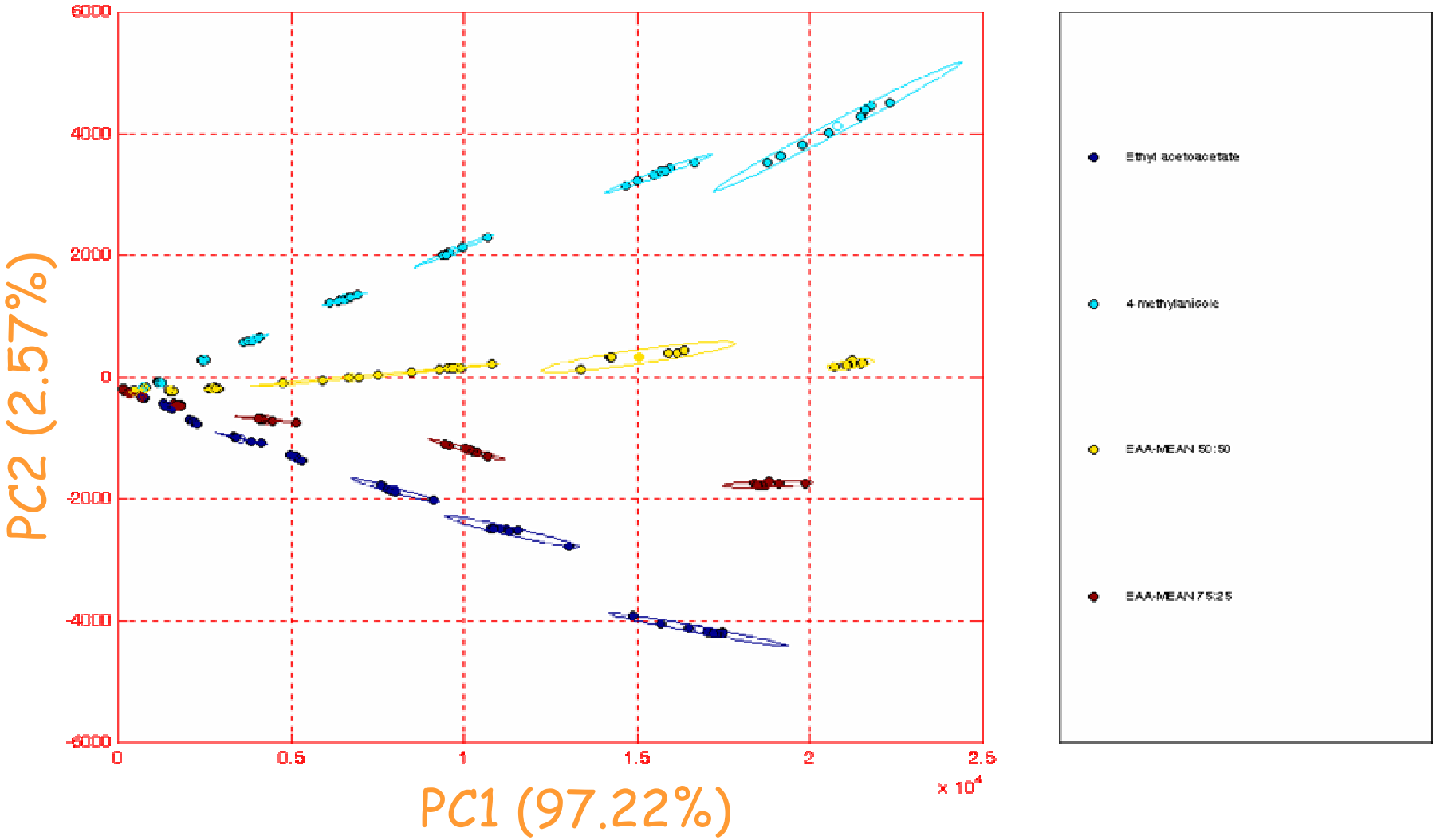
Predict location of a mixture

Get to a desired point by mixing

Crucial: Must have non-1-1 transformations

⇨ how do chemicals mix???

Example of results for mixing
(notice both kinds of linearity!)



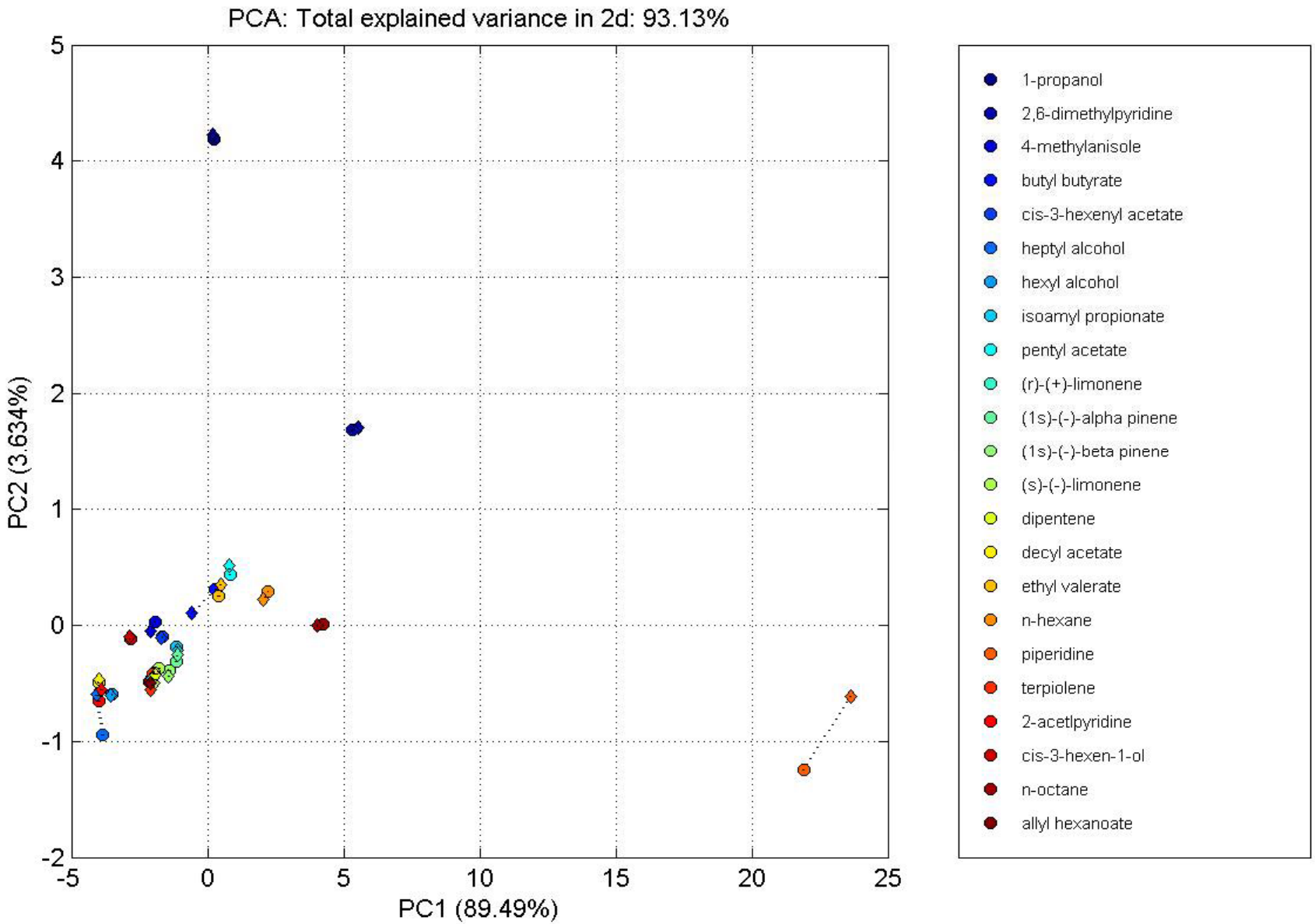
Mapping one eNose to another

(with Oded Shaham)

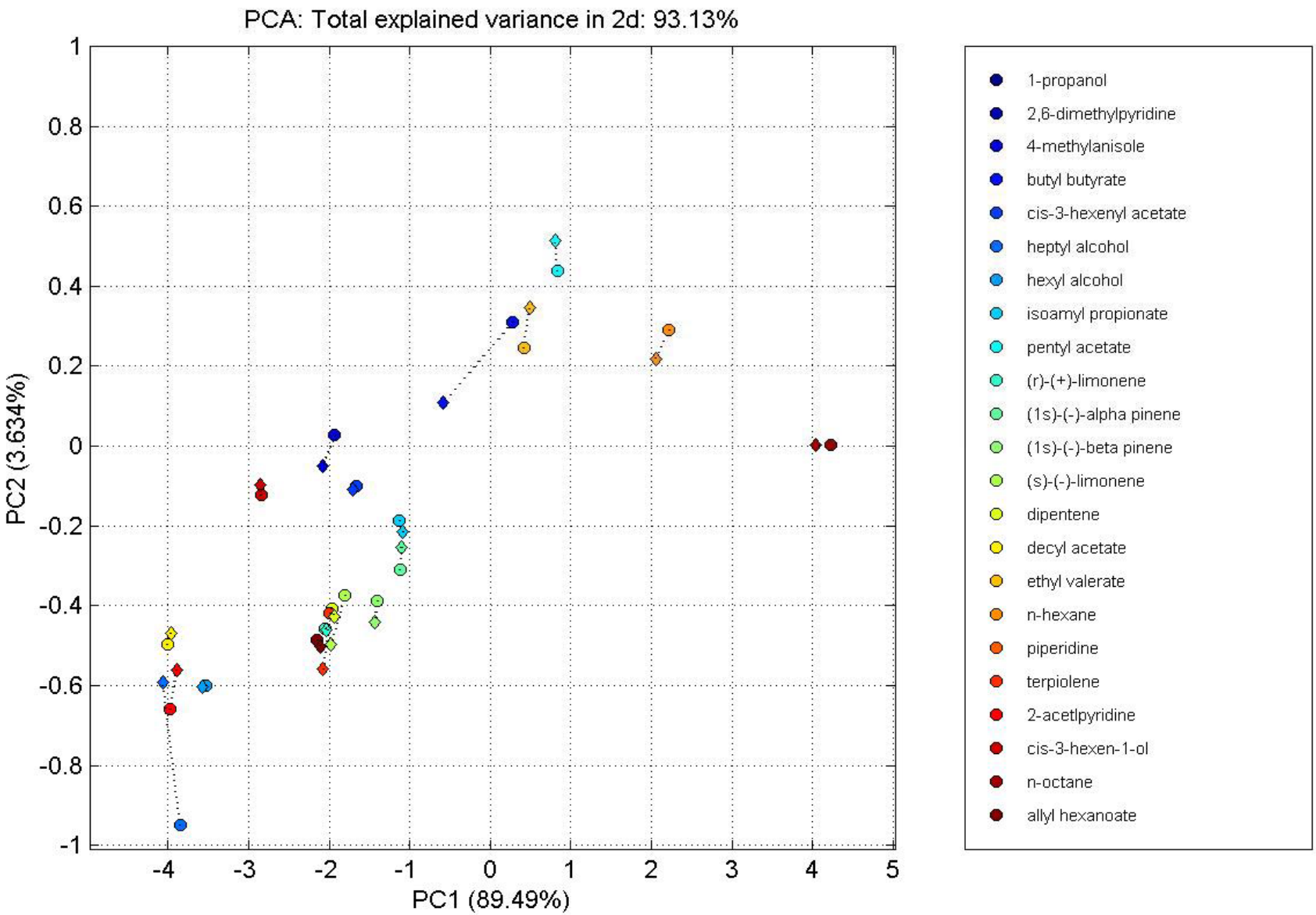
We have been able to map the 8 QMB sensors of MosesII to the 32 conducting polymers (CP) sensors of the Cyranose

Method: tessellation-based linear interpolation

Circles: actual samples Diamonds: predictions



Zoom-in on the dense area



Ideas for advanced research

- Flexibility of choice based on requirements:
  - hardware (methods improve with age…)
  - palette (size, contents, etc.)
  - tolerance (error, mixing limitations, etc.)
- Non-uniform palette techniques:
  - multi-tier mixing
  - varying reservoir sizes
  - feedback-driven mixing
    (e.g., by personalization)

Lots of work still to be done

Most important: careful and detailed investigation of human panel space…