Shogun Toolbox Days 2013

July 12th 2013 Workshop Schedule

11:00 - 11:30 Welcome: Machine learning *speed-dating* accompanied by coffee.
11:30 - 12:30 Introduction to machine learning and applications (Gunnar).
12:30 - 13:00 Shogun introduction, features and installation (Sören).
13:00 - 14:00 *Lunch break*.
14:00 - 15:00 Support Vector Machines / Multiple Kernel Learning (Sören).
15:00 - 16:00 Gaussian Processes / Kernel Statistical Tests (MMD/HSIC) (Heiko).
16:00 - 16:30 *Coffee break*.
16:30 - 17:00 Discussion: usability & development-process of Shogun
17:00 - 17:30 Dimension Reduction (Sergey).
17:30 - 18:00 Structured Output Learning (Fernando).
18:00 - 18:30 (Latent) Structured Output SVM in practice (Viktor).
18:30 - 19:00 Discussion: Future of Shogun

Grand Finale: **BBQ & Drinks**

Memorial Sloan-Kettering Cancer Center

The Best Cancer Care. Anywhere.

Introduction to Machine Learning in Science and Engineering

Gunnar Rätsch
Memorial Sloan-Kettering Cancer Center
New York, USA
http://raetschlab.org/

1st Shogun Developer Meeting
c-base Berlin

Roadmap

Part I

- Motivating Examples & Background
- Boosting & SVMs & some Applications

Part II

- Something more technical

Part III

- Some current work

Rationale: Let computers learn to automate processes and to understand highly complex data

Example 1: Spam Classification

From: smartballlottery@hf-uk.org
Subject: Congratulations
Date: 16. December 2004 02:12:54 MEZ

LOTTERY COORDINATOR,
INTERNATIONAL PROMOTIONS/PRIZE AWARD DEPARTMENT.
SMARTBALL LOTTERY, UK.

DEAR WINNER,

WINNER OF HIGH STAKES DRAWS

Congratulations to you as we bring to your notice, the results of the the end of year, HIGH STAKES DRAWS of SMARTBALL LOTTERY UNITED KINGDOM. We are happy to inform you that you have emerged a winner under the HIGH STAKES DRAWS SECOND CATEGORY,which is part of our promotional draws. The draws were held on15th DECEMBER 2004 and results are being officially announced today. Participants were selected through a computer ballot system drawn from 30,000 names/ email addresses of individuals and companies from Africa, America, Asia, Australia,Europe, Middle East, and Oceania as part of our International Promotions Program.

…

From: manfred@cse.ucsc.edu
Subject: ML Positions in Santa Cruz
Date: 4. December 2004 06:00:37 MEZ

We have a Machine Learning position
at Computer Science Department of
the University of California at Santa Cruz
(at the assistant, associate or full professor level).

Current faculty members in related areas:
Machine Learning: DAVID HELMBOLD and MANFRED WARMUTH
Artificial Intelligence: BOB LEVINSON
DAVID HAUSSLER was one of the main ML researchers in our department. He now has launched the new Biomolecular Engineering department at Santa Cruz

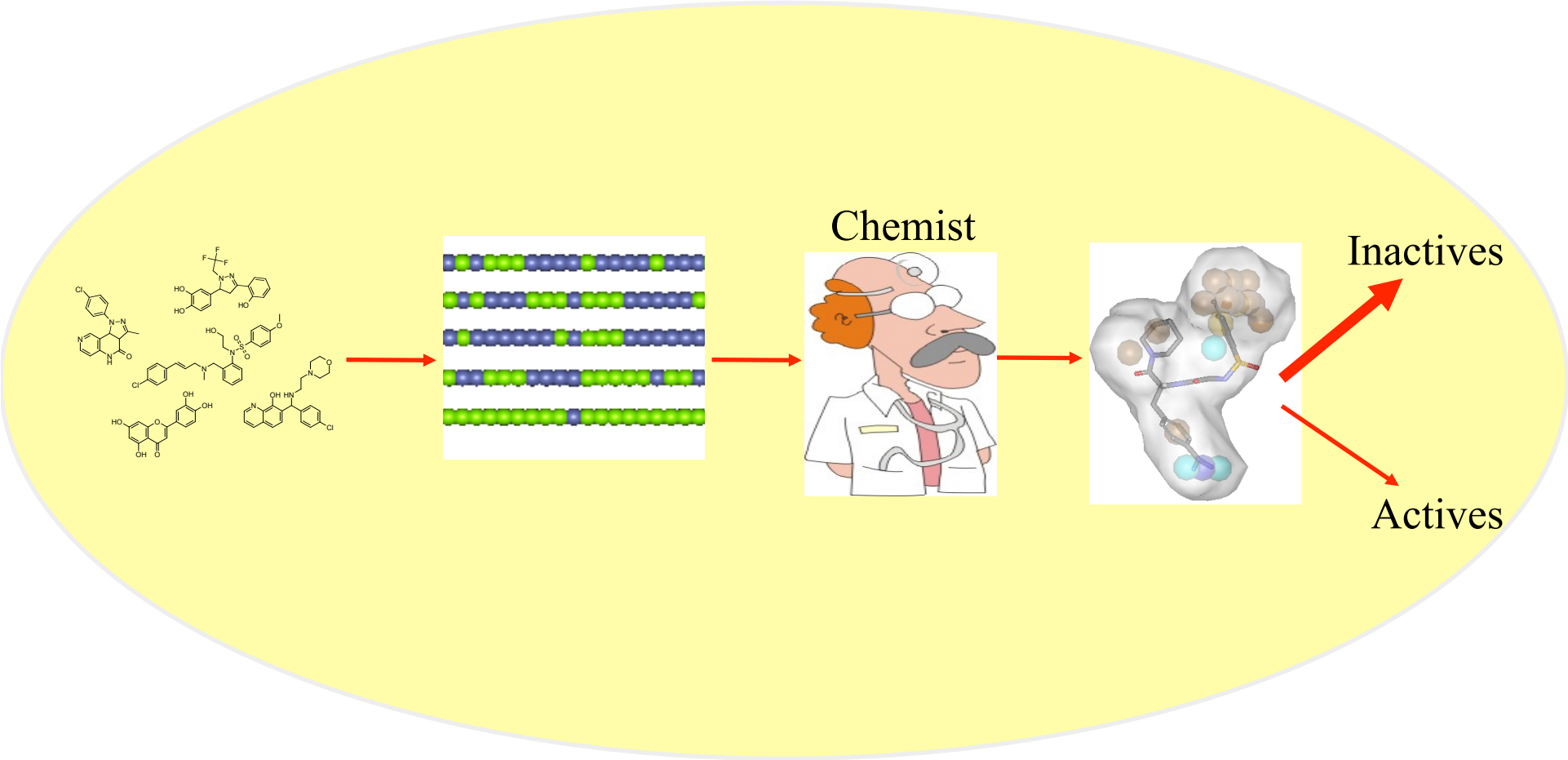
There is considerable synergy for Machine Learning at Santa Cruz:
-New department of Applied Math and Statistics with an emphasis on Bayesian Methods http://www.ams.ucsc.edu/
-- New department of Biomolecular Engineering http://www.cbse.ucsc.edu/

…

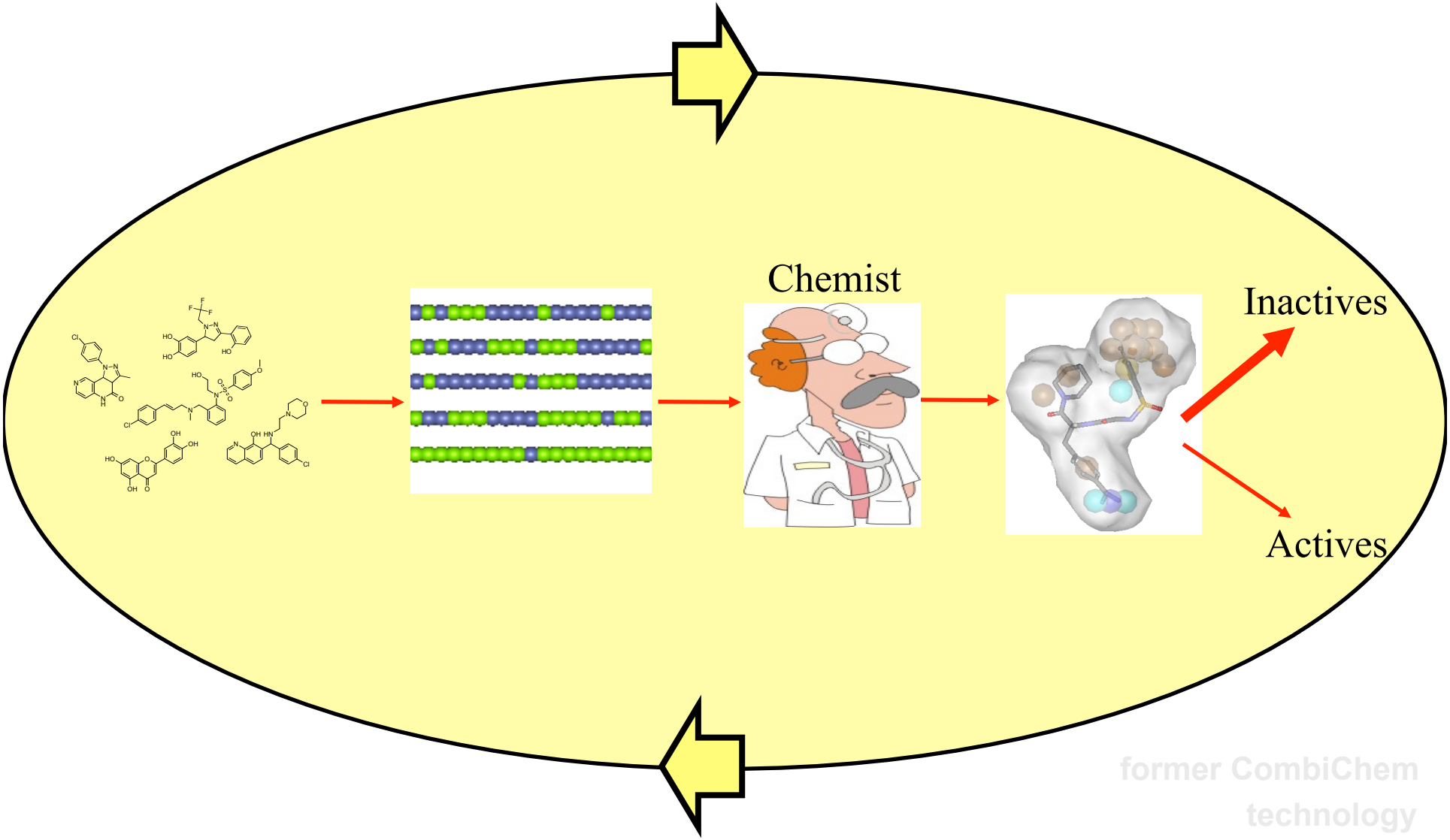
Goal: Classify emails into spam / no spam
How? Learn from previously classified emails!

Training: analyze previous emails
Application: classify new emails

Example 2: Drug Design

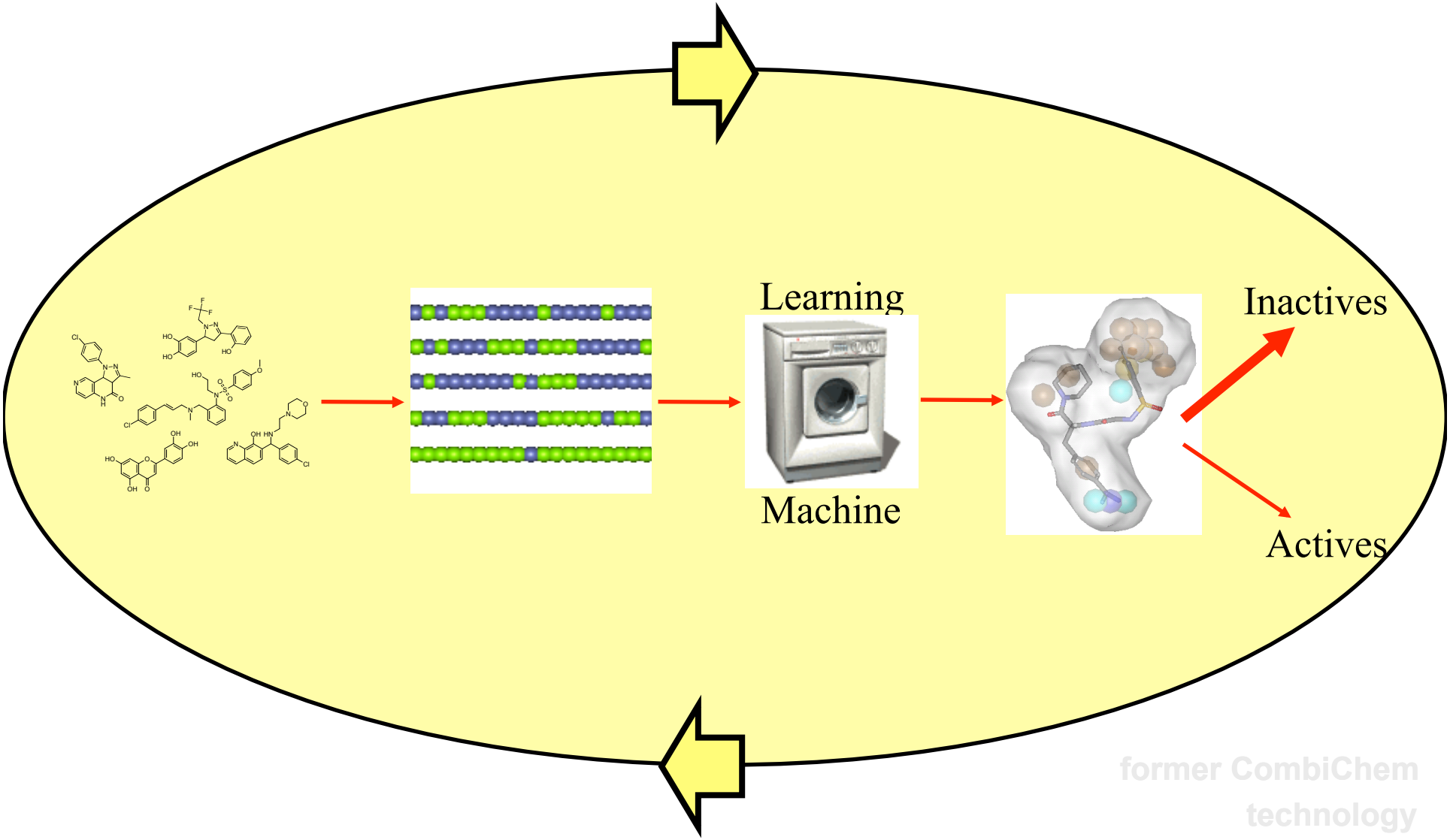


The Drug Design Cycle



former CombiChem technology

The Drug Design Cycle



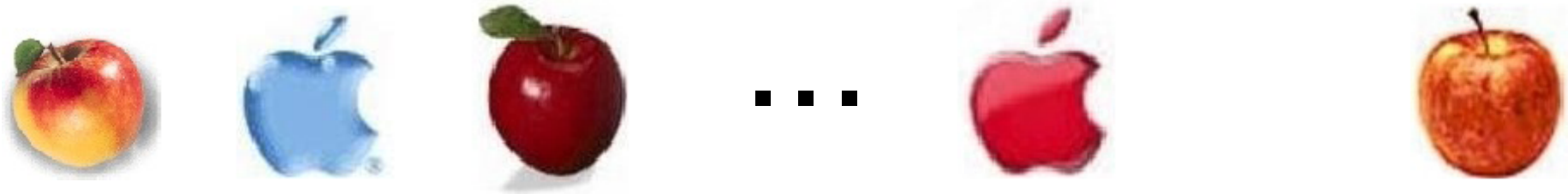
former CombiChem technology

Example 3: Face Detection

Premises for Machine Learning

- Supervised Machine Learning
  - Observe N training examples with label
    $$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$$
  - Learn function $f : \mathbf{x} \longrightarrow y$
  - Predict label of unseen example $f(\mathbf{x})$
- Examples generated from statistical process
- Relationship between features and label
- **Assumption:** unseen examples are generated from same or similar process

Problem Formulation



Natural	Plastic	Natural		Plastic	?
+1	-1	+1		-1	

The "World":

- Data $\{(\mathbf{x}_n, y_n)\}_{n=1}^N, \mathbf{x}_n \in \mathbb{R}^d, y_n \in \{\pm 1\}$
- Unknown Target Function $y = f(\mathbf{x})$
- Unknown Distribution $\mathbf{x} \sim p(\mathbf{x})$
- Objective Given new $\mathbf{x}$, predict y

Problem: $P(\mathbf{x}, y)$ is unknown

Problem Formulation

The 'Model'

Hypothesis class: $\mathcal{H} = \left\{ h \mid h : \mathbf{R}^d \to \{\pm 1\} \right\}$

Loss: $l(y, h(\mathbf{x}))$ (e.g. $\mathbf{I}[y \neq h(\mathbf{x})]$)

Objective: Minimize the true (expected) loss – "generalization error"

$$h^* = \text{argmin}_{h \in \mathcal{H}} \; L(h) \text{ with } \boxed{L(h) := \mathbf{E}_{\mathbb{X} \times \mathbb{Y}} \; l(\mathbb{Y}, h(\mathbb{X}))}$$

Problem: Only have a data sample available, $P(\mathbf{x}, y)$ is unknown!

Solution: Find empirical minimizer

$$\hat{h}_N = \text{argmin}_{h \in \mathcal{H}} \; \frac{1}{N} \sum_{n=1}^{N} l(y_n, h(\mathbf{x}_n))$$

Example: Natural vs. Plastic Apples

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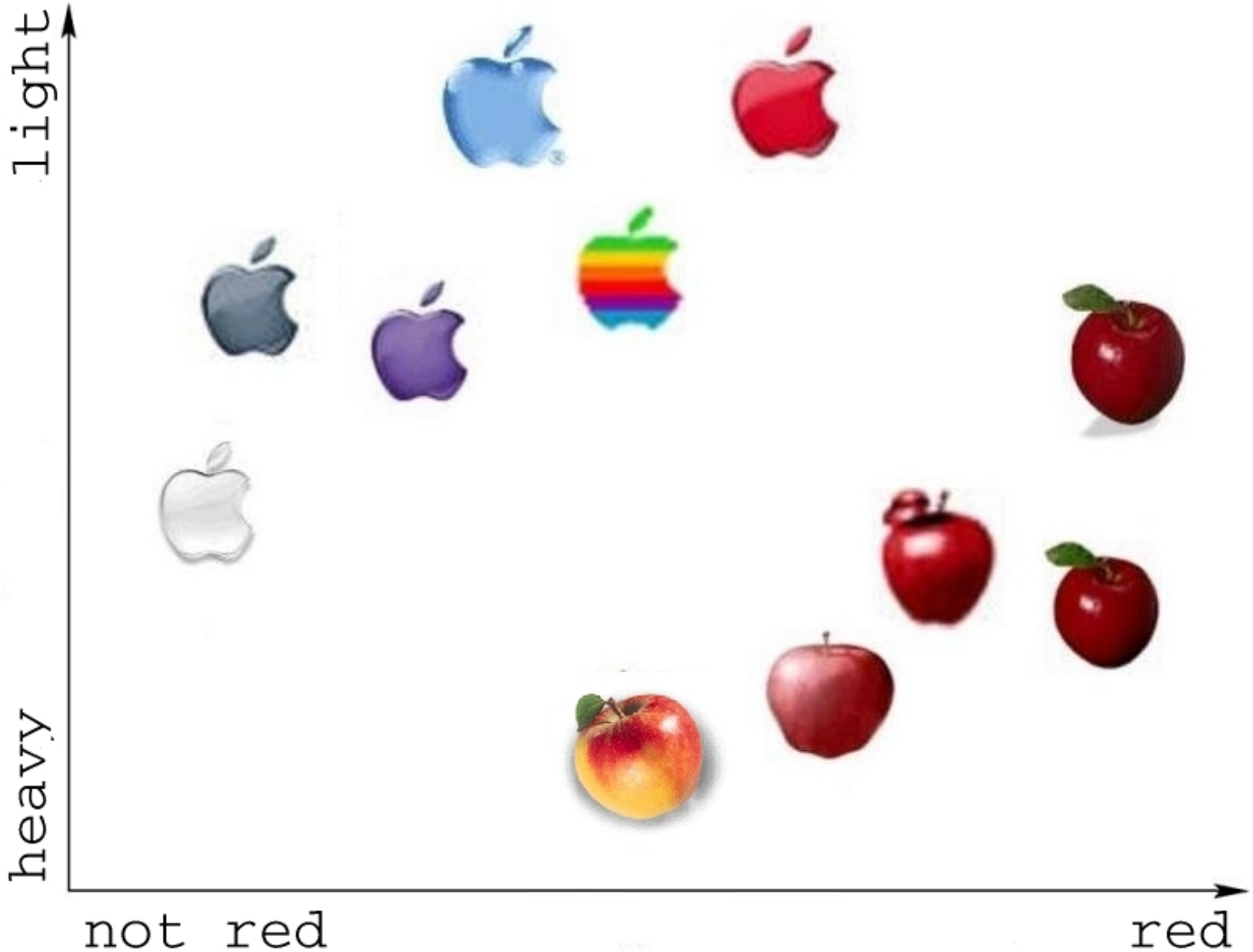

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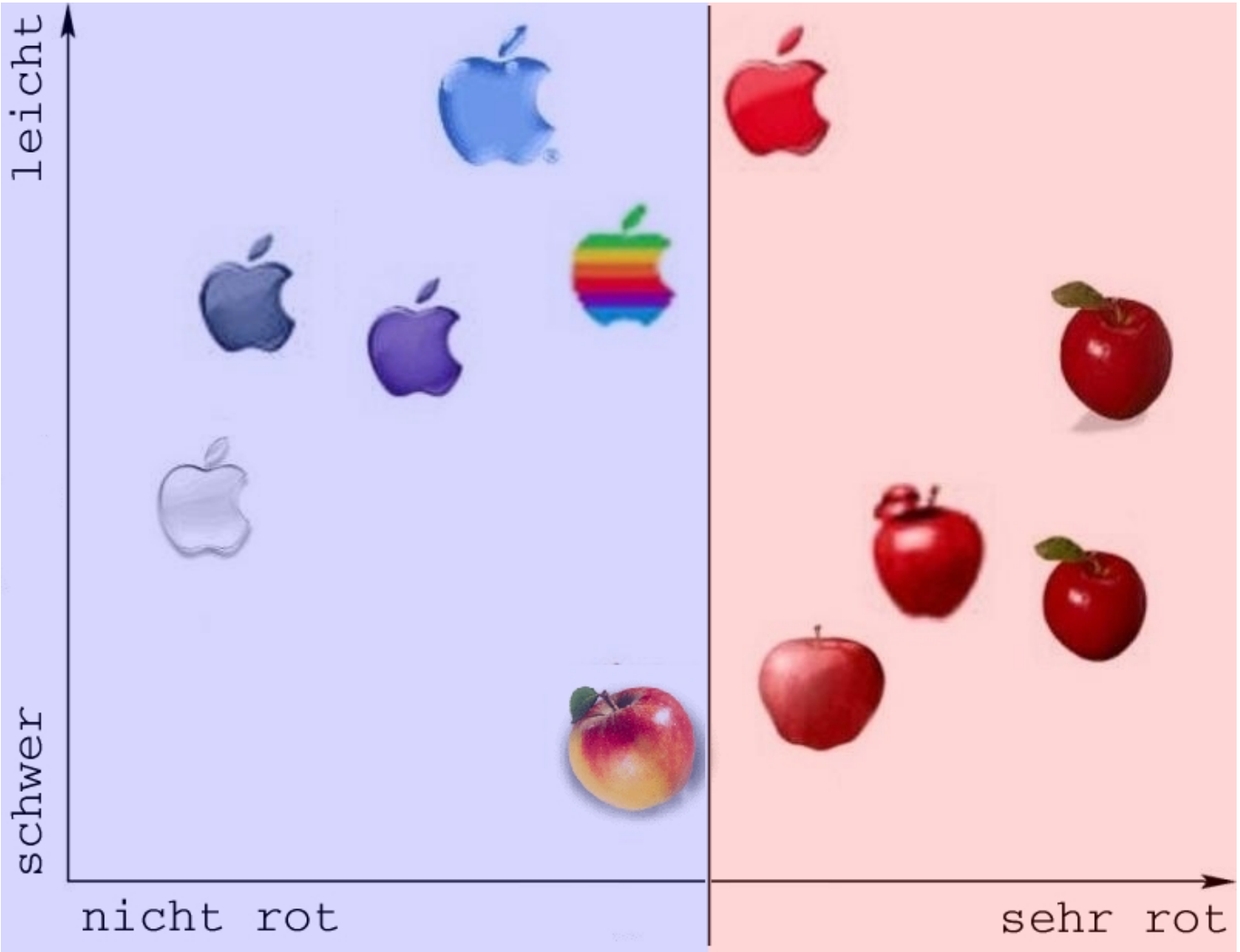
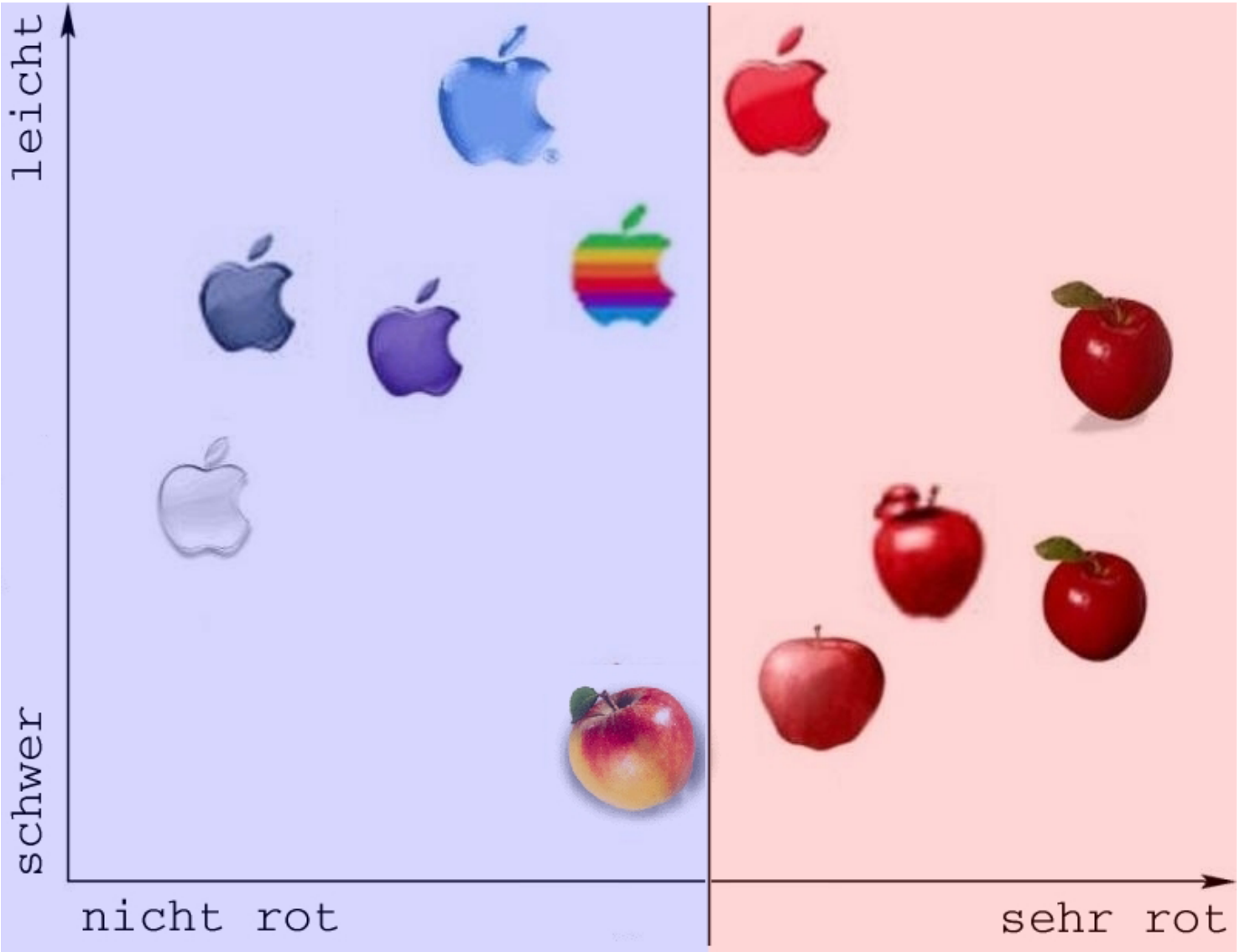


AdaBoost (Freund & Schapire, 1996)

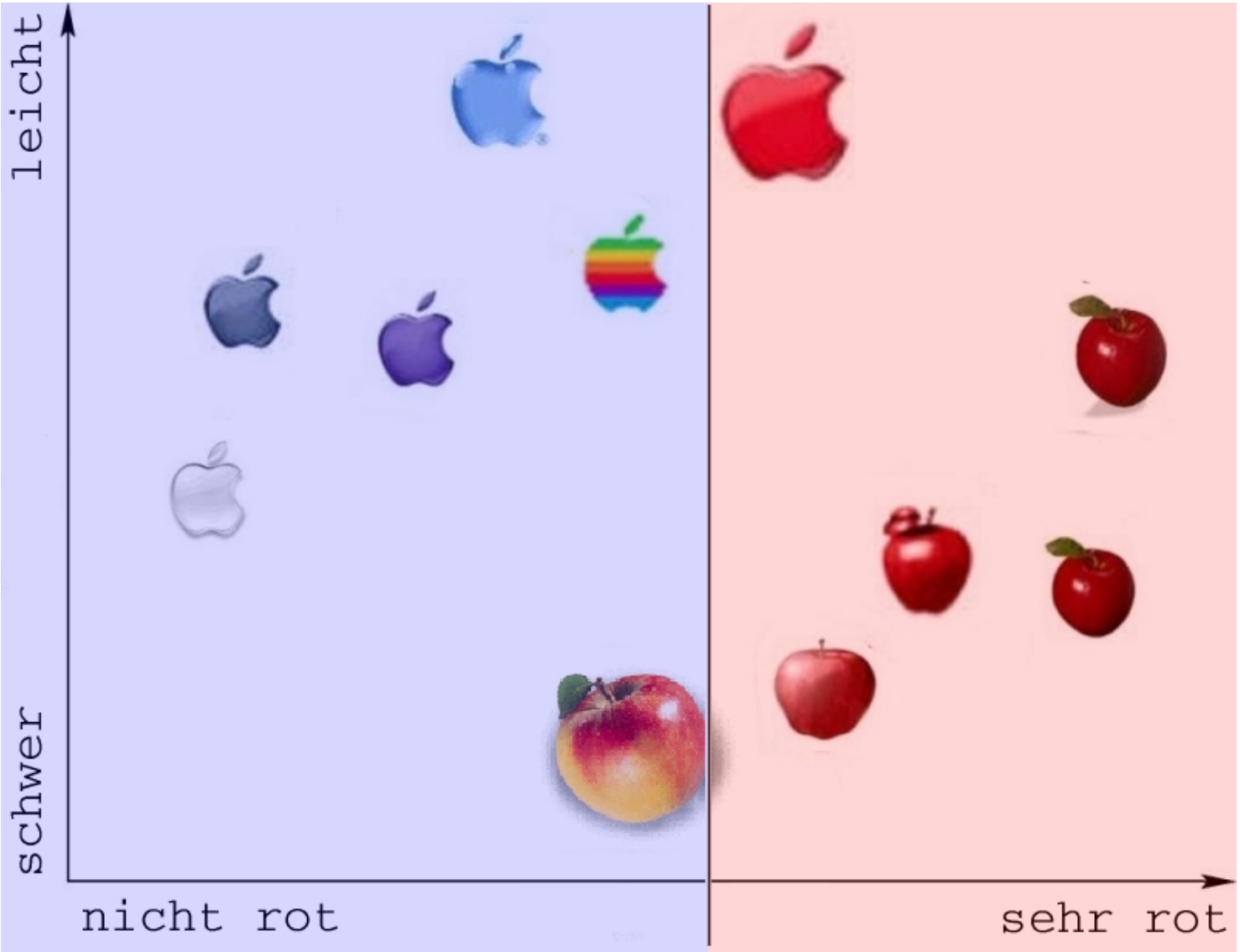
- **Idea:**
  - Use simple many “rules of thumb”
  - Simple hypotheses are not perfect!
  - Hypotheses combination => increased accuracy
- **Problems**
  - How to generate different hypotheses?
  - How to combine them?
- **Method**
  - Compute distribution $d_1, \ldots, d_N$ on examples
  - Find hypothesis on the weighted sample
  - Combine hypotheses $h_1, \ldots, h_J$ linearly:

$$f(\mathbf{x}) = \sum_{j=1}^{J} \alpha_j h_j(\mathbf{x})$$

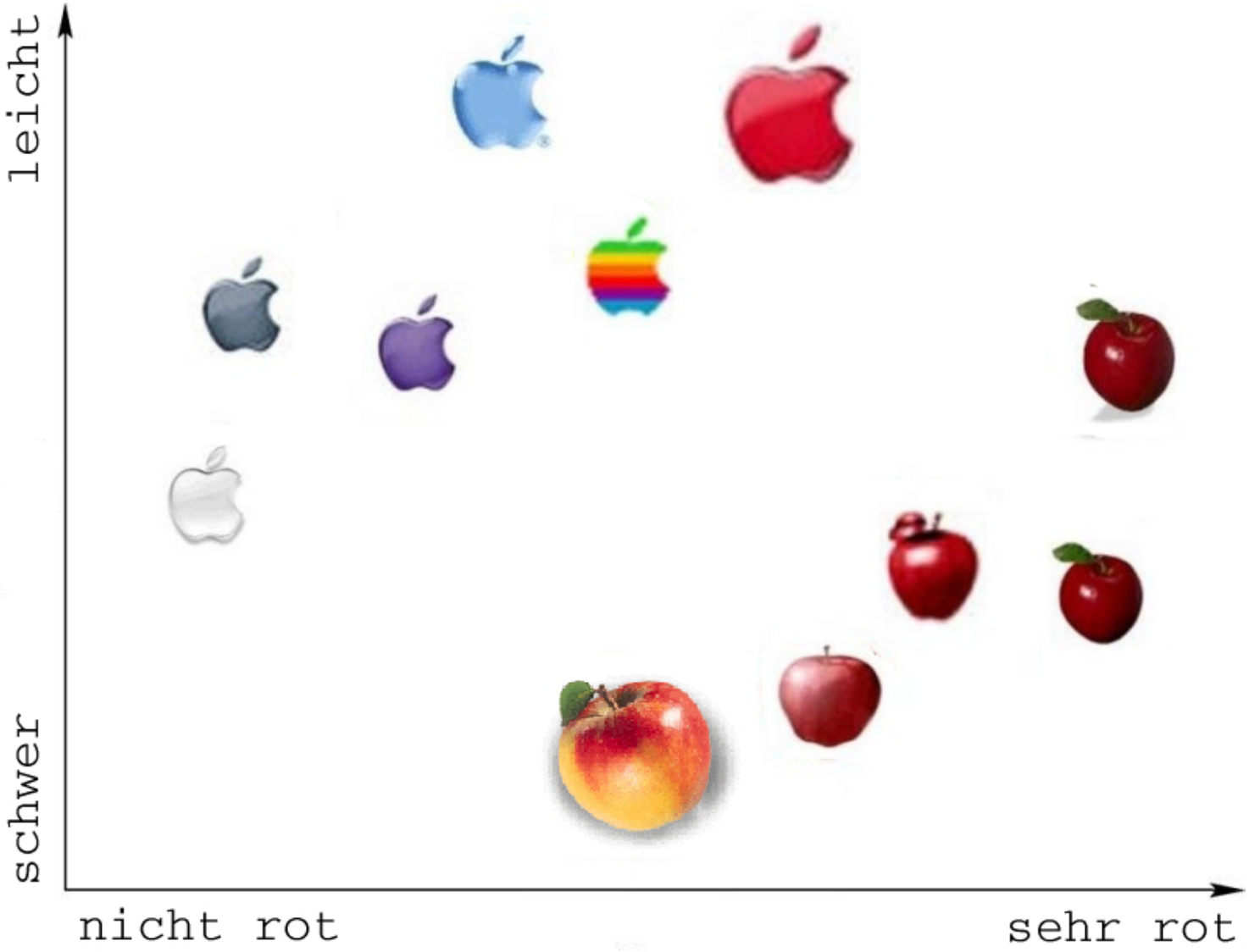
Boosting: 1st iteration (simple hypothesis)



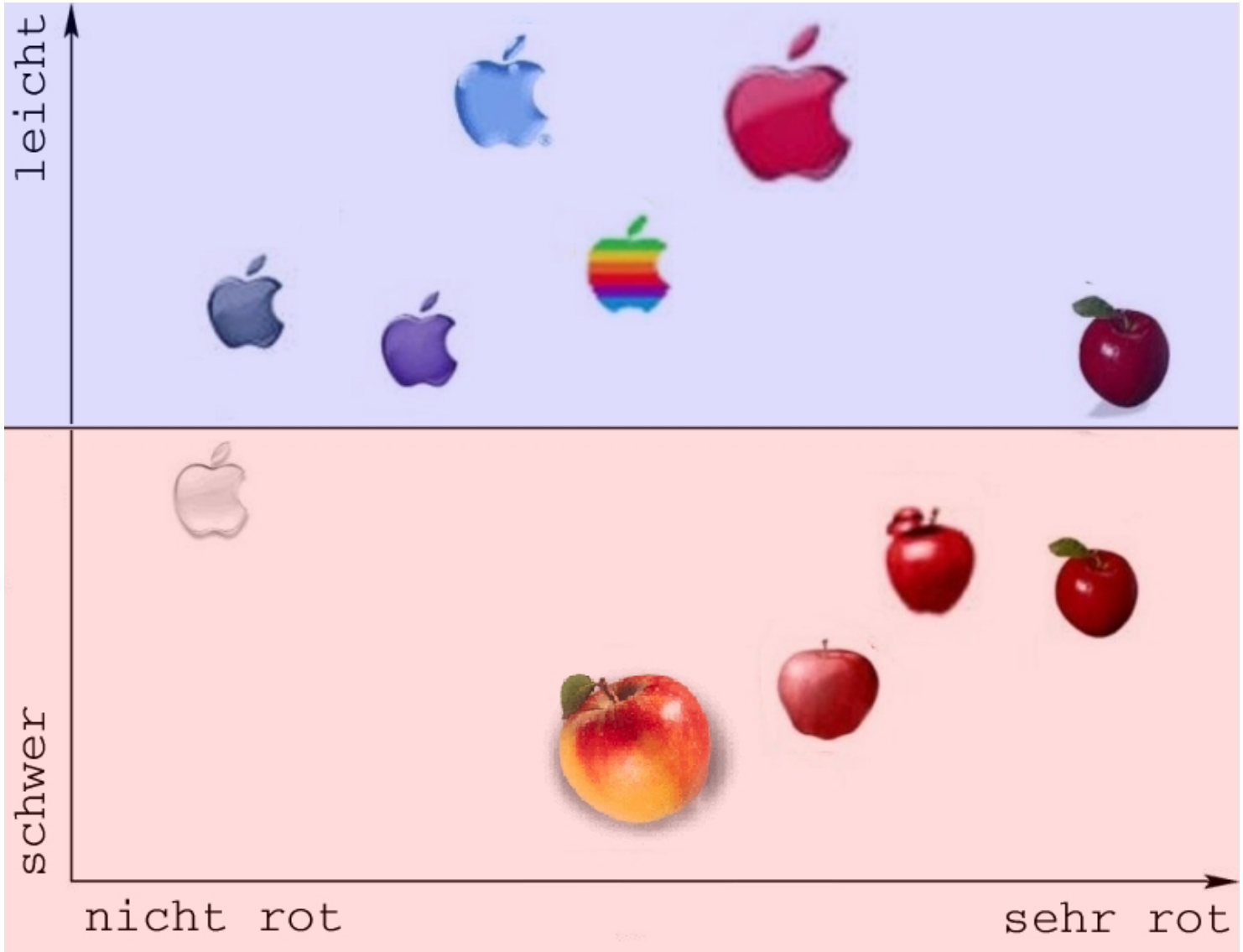
Boosting: recompute weighting



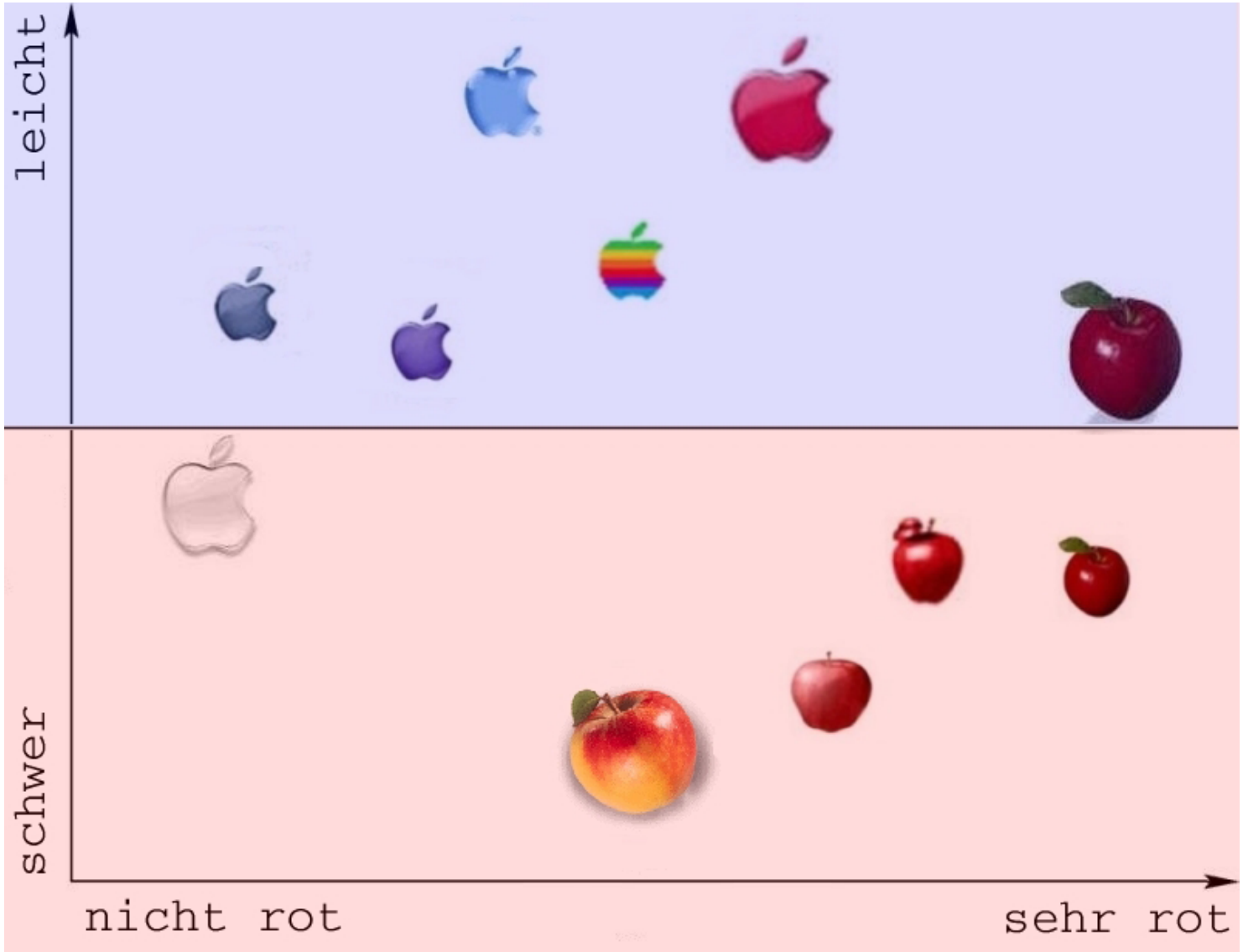
Boosting: 2nd iteration



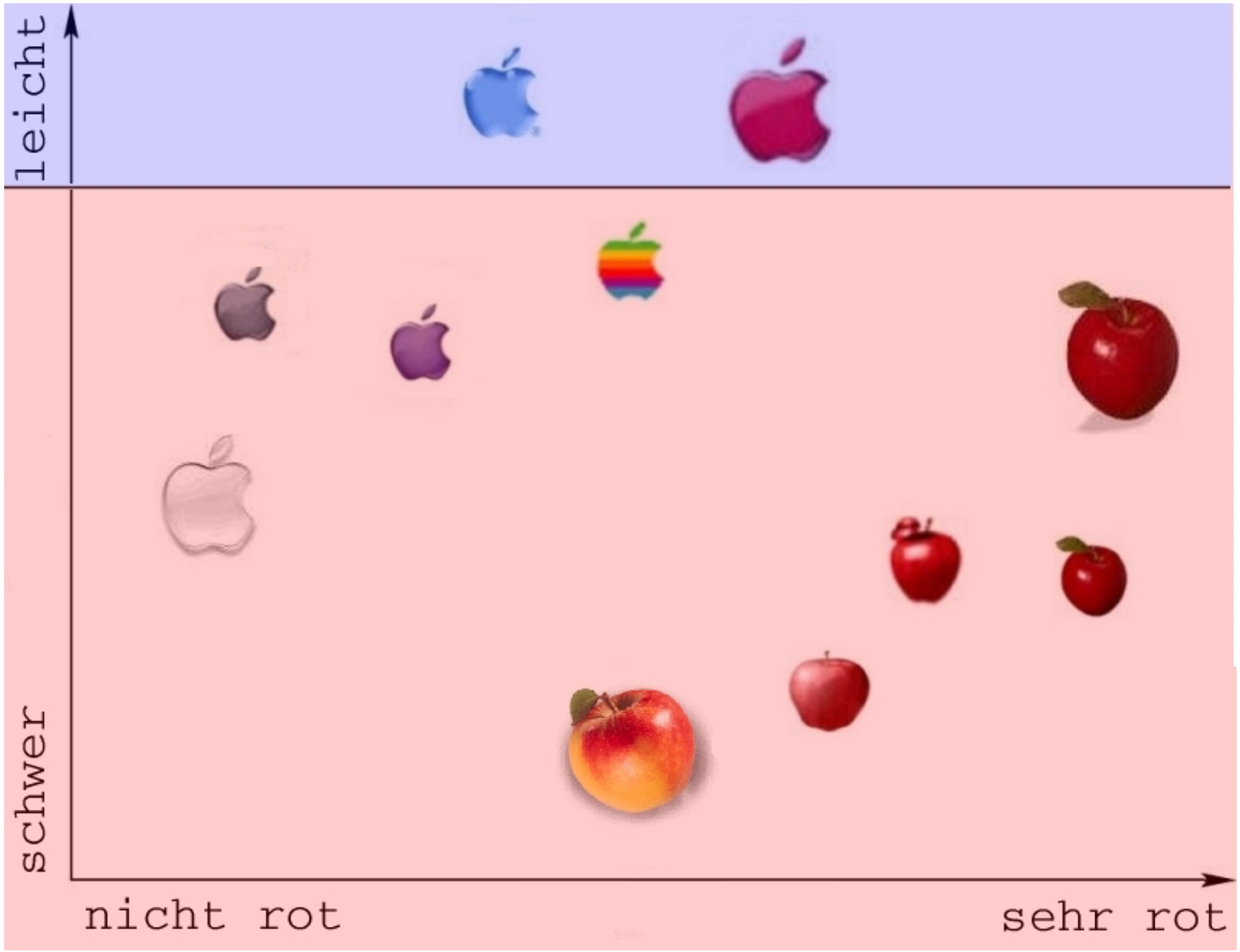
Boosting: 2nd hypothesis



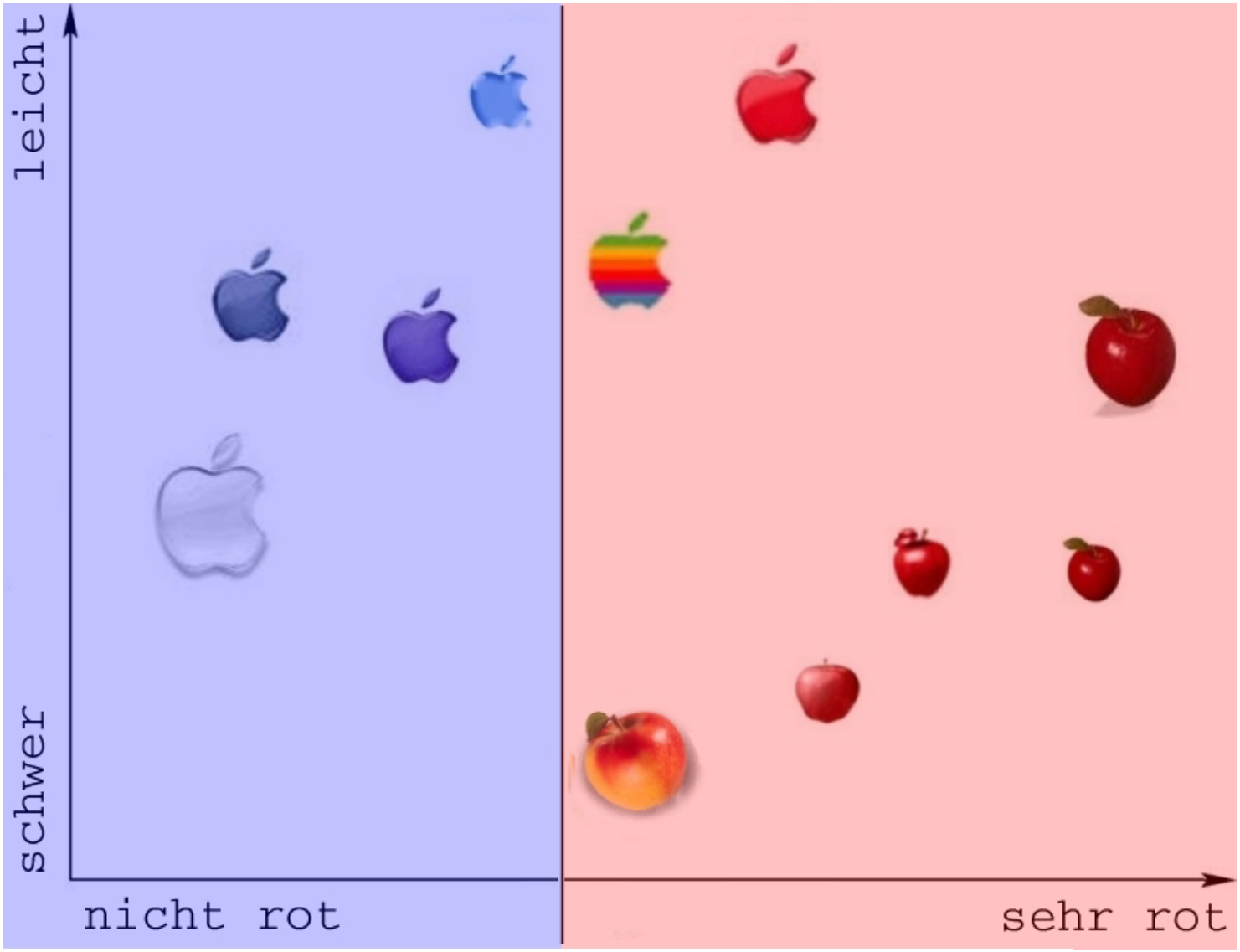
Boosting: recompute weighting



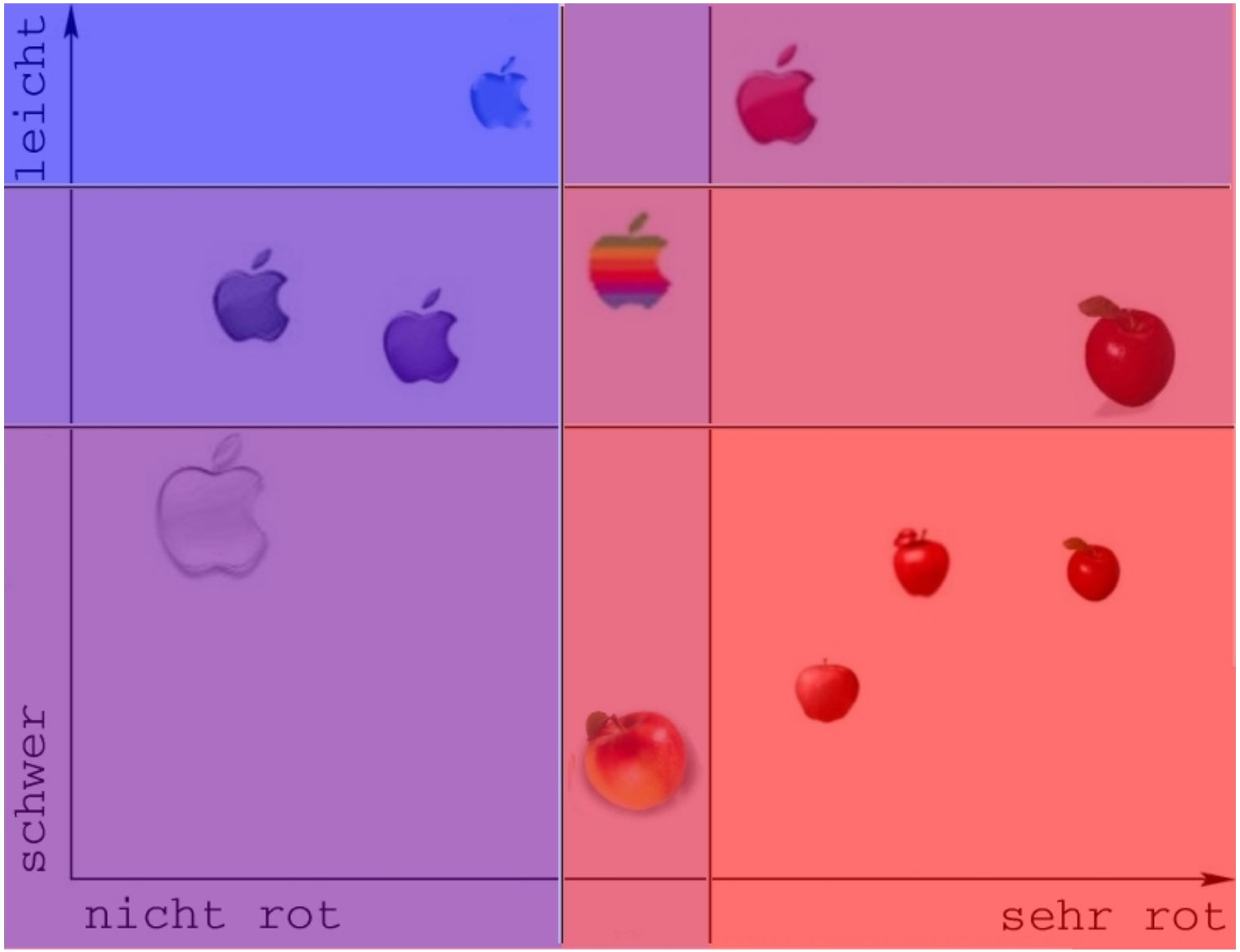
Boosting: 3rd hypothesis



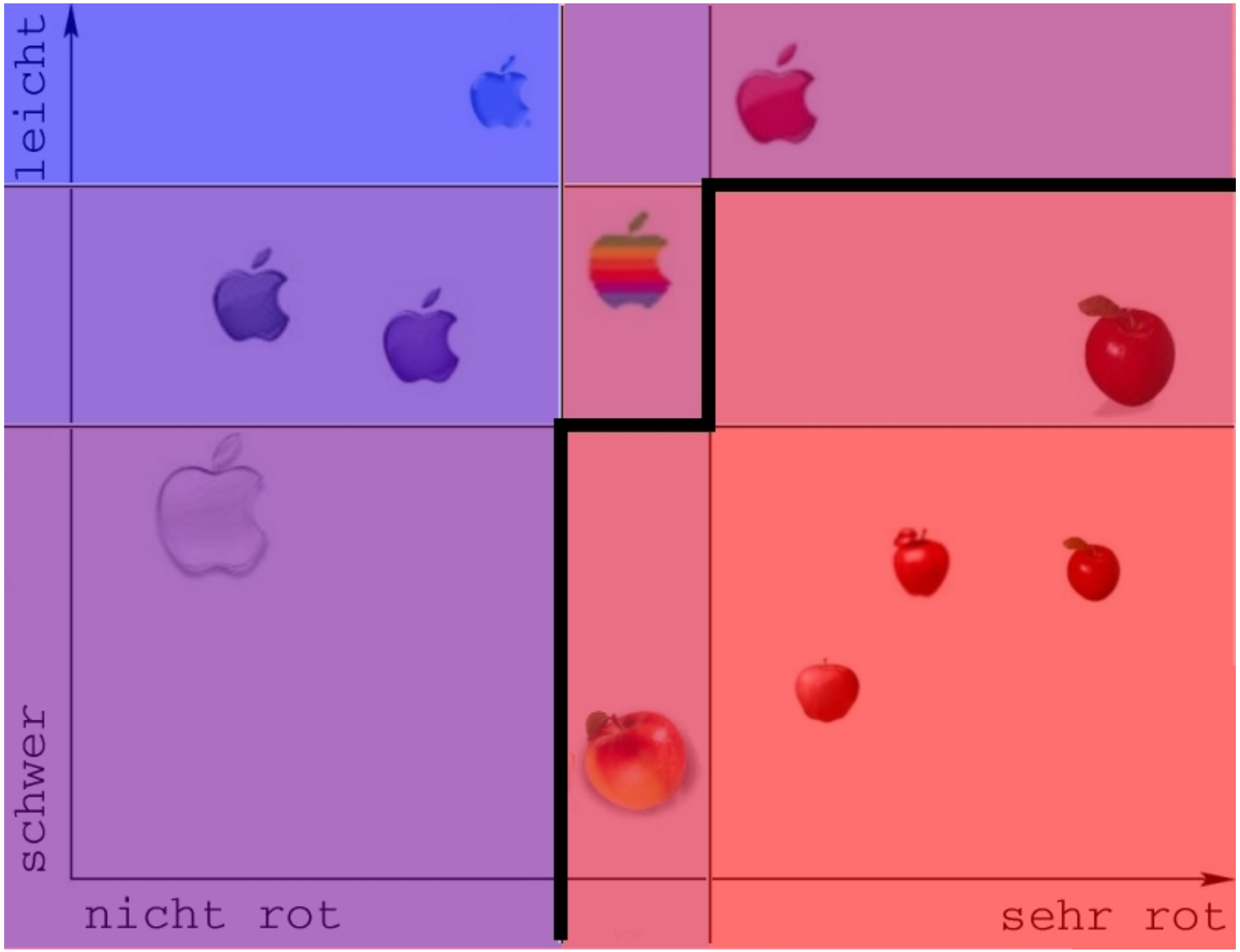
Boosting: 4rd hypothesis



Boosting: combination of hypotheses



Boosting: decision



AdaBoost Algorithm

Input: N examples $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$
Initialize: $d_n^{(1)} = 1/N$ for all $n = 1 \ldots N$
Do for $t = 1, \ldots, T$,

1. Train base learner according to example distribution $\mathbf{d}^{(t)}$ and obtain hypothesis $h_t : \mathbf{x} \mapsto \{\pm 1\}$.
2. compute weighted error $\epsilon_t = \sum_{n=1}^{N} d_n^{(t)} \mathbf{I}(y_n \neq h_t(\mathbf{x}_n))$
3. compute hypothesis weight $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$
4. update example distribution

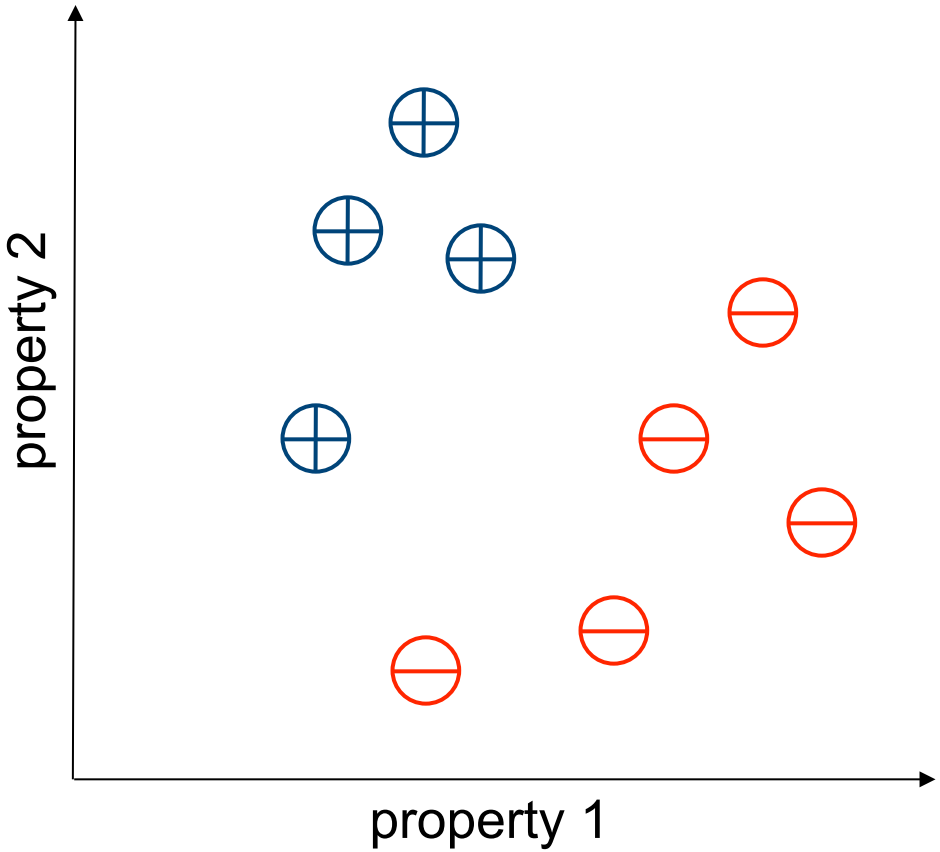
$$d_n^{(t+1)} = d_n^{(t)} \exp\left(-\alpha_t y_n h_t(\mathbf{x}_n)\right) / Z_t$$

Output: final hypothesis $f_{\mathsf{Ens}}(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})$

AdaBoost algorithm

- Combination of
  - Decision stumps/trees
  - Neural networks
  - Heuristic rules
- Many improvements
  - Robustness, multiclass, speed, …
- Further reading
  - http://www.boosting.org/tutorials
  - http://www.mlss.cc

Linear Separation



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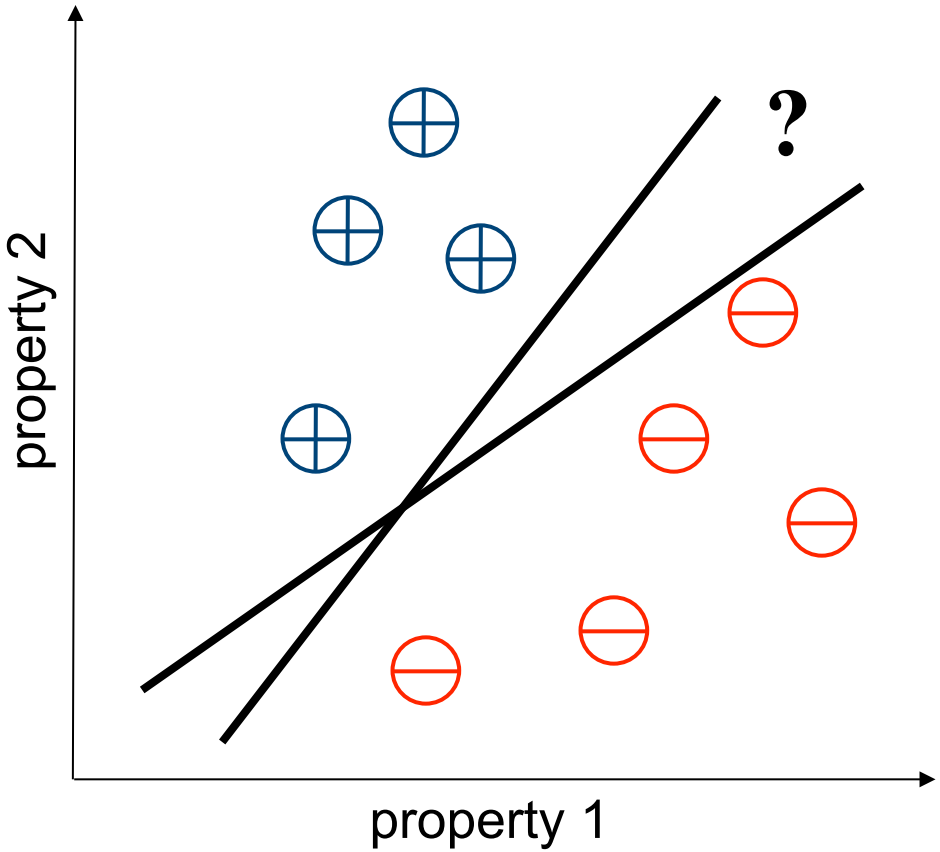
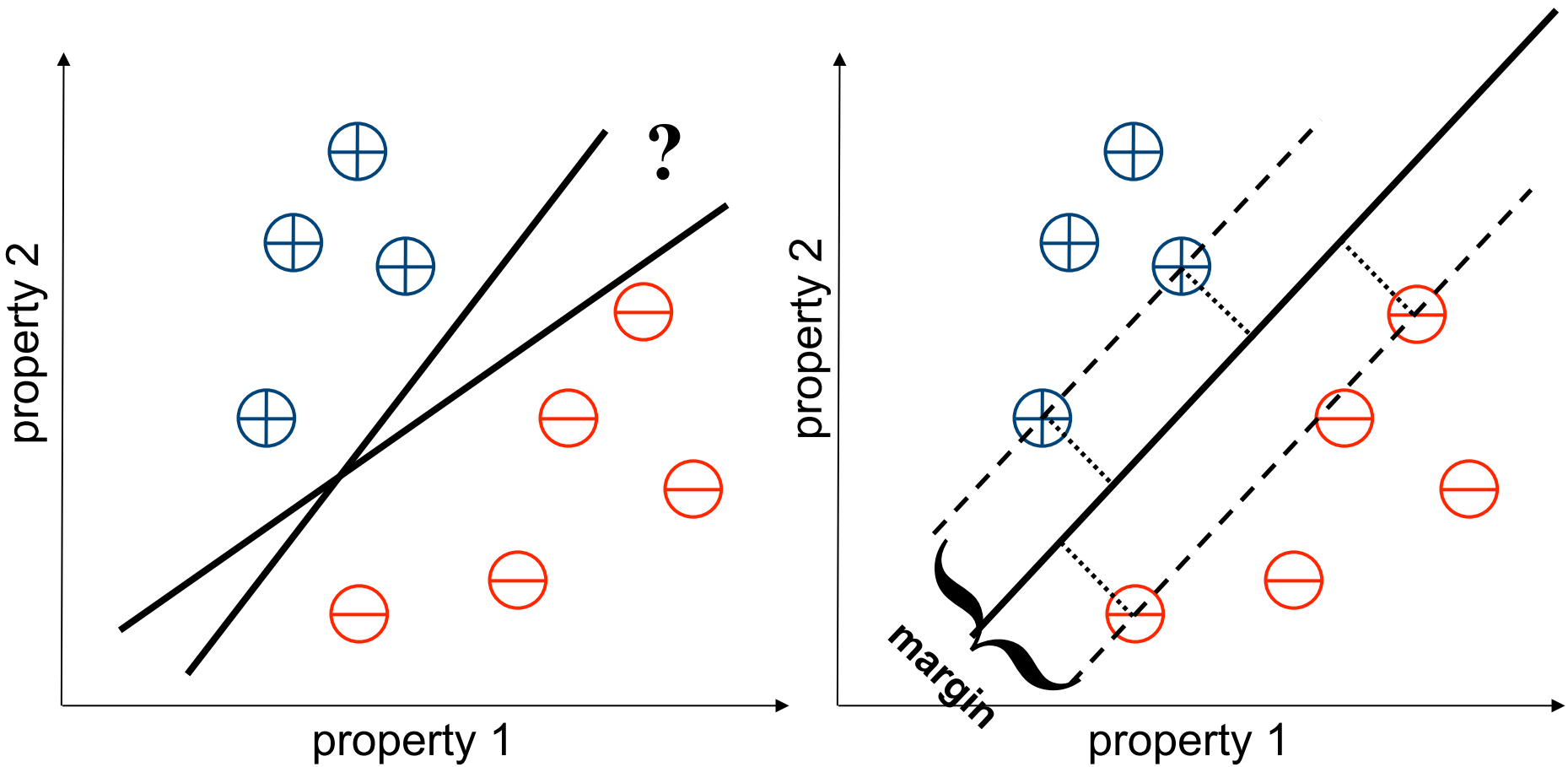


Linear Separation with Margins



large margin => good generalization

Large Margin Separation

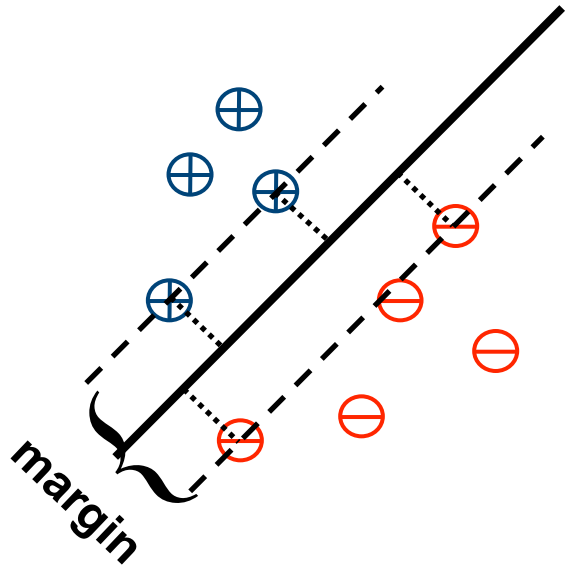
Idea:

- Find hyperplane $f(\mathbf{x}) = (\mathbf{w} \cdot \mathbf{x})$ that maximizes margin

$$f(\mathbf{x}^+) - f(\mathbf{x}^-)$$

(with $\|\mathbf{w}\|_2 = 1$)

- Use $\mathrm{sgn}(f(\mathbf{x}) + b)$ for prediction

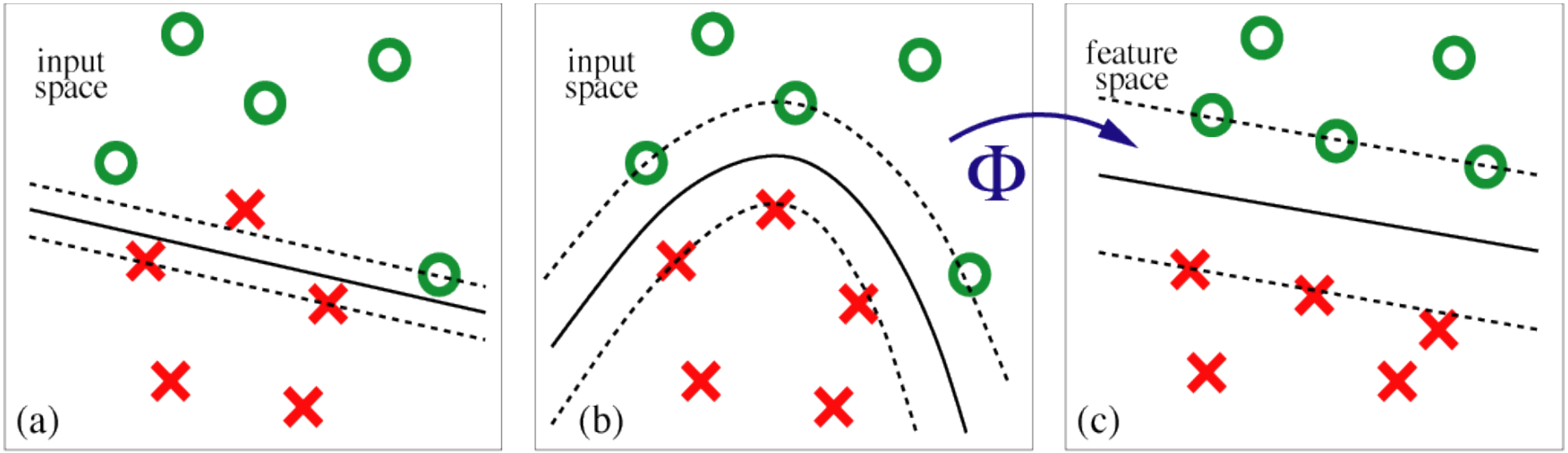


Solution:

- Linear combination of examples $\mathbf{w} = \sum_{n=1}^{N} \alpha_n \mathbf{x}_n$
- many α's are zero
- **Support Vector Machines**

  $\Rightarrow$ **Demo**

Kernel Trick



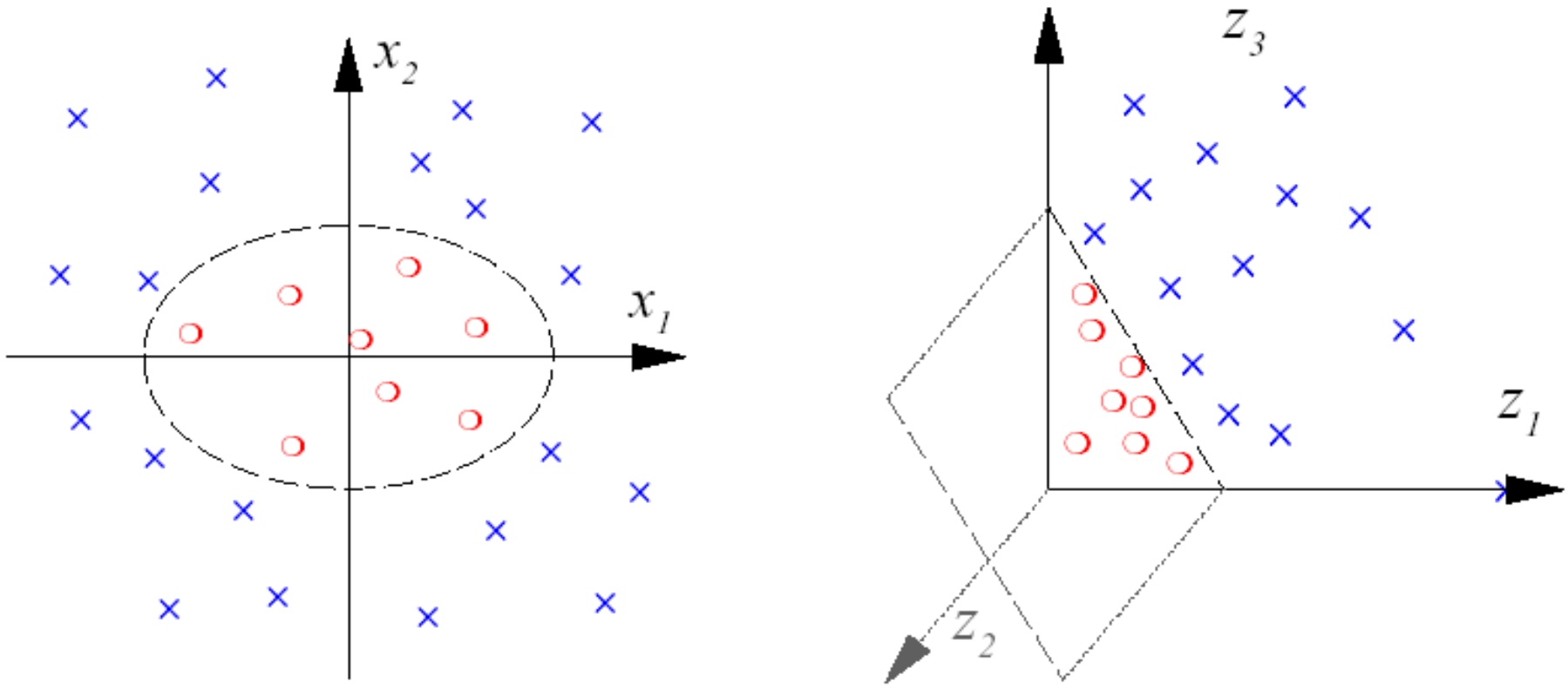
Linear in input space | **Non-linear in input space** ⇐ **Linear in feature space**

$$k(\mathbf{x}, \mathbf{x}') = (\Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}'))$$

Example: Polynomial Kernel

$$\Phi : \mathbb{R}^2 \to \mathbb{R}^3$$

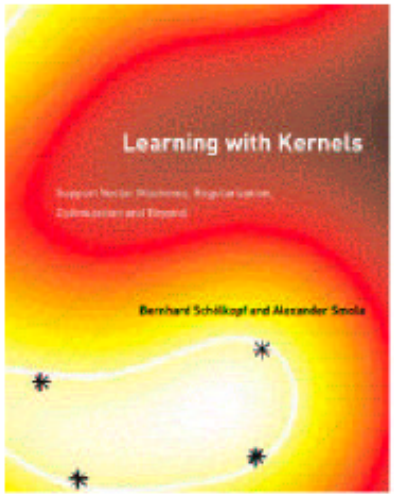
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)$$



$$k(\mathbf{x}, \mathbf{x}') = (\Phi(\mathbf{x}) \cdot \Phi(\mathbf{x}')) = (\mathbf{x} \cdot \mathbf{x}')^2$$

Support Vector Machines

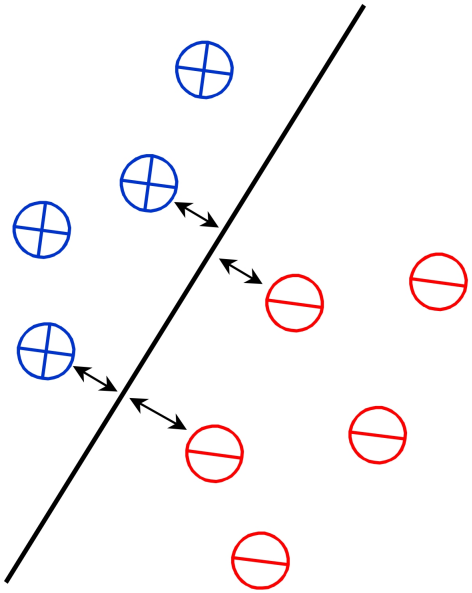
- **Demo:** Gaussian Kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|}{2\sigma^2}\right)$
- Many other algorithms can use kernels
- Many other application specific kernels



For further information, cf.
http://www.kernel-machines.org,
http://www.learning-with-kernels.org

Capabilities of Current Techniques

- Theoretically & algorithmically well understood:
  - **Classification with few classes**
  - Regression (real valued)
  - Novelty Detection



Bottom Line: *Machine Learning works well for relatively simple objects with simple properties*

- Recent Research
  - Complex objects
  - Many classes
  - Complex learning setup (active or transfer learning)
  - Prediction of complex properties

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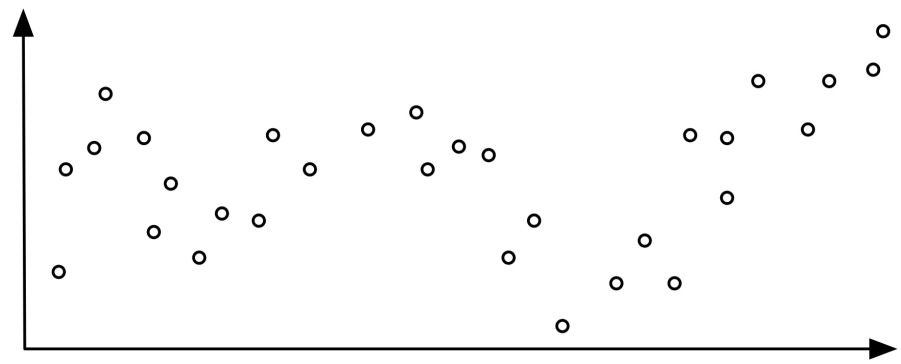

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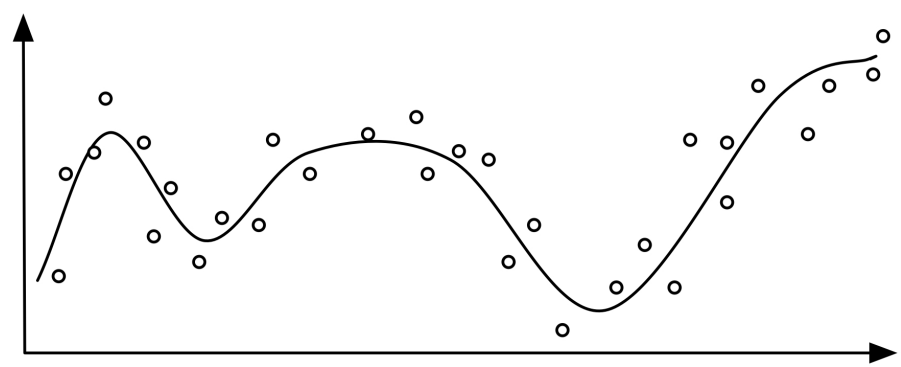

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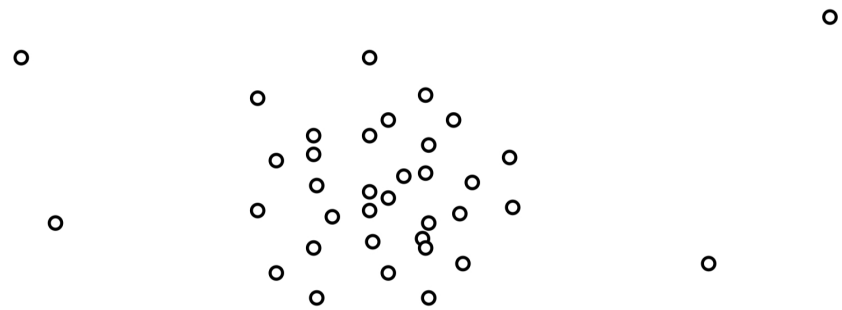

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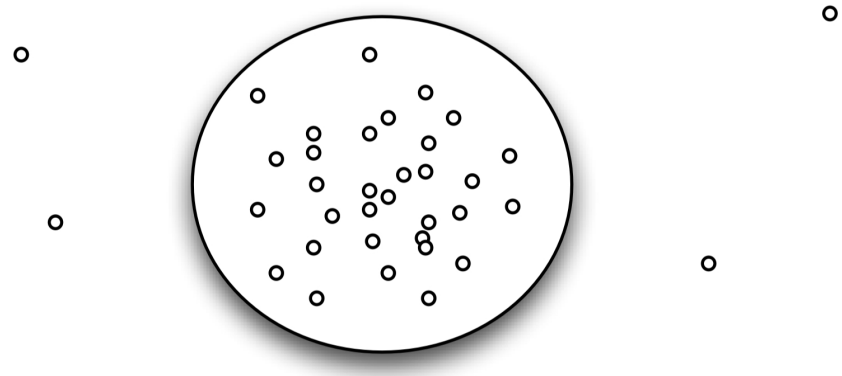

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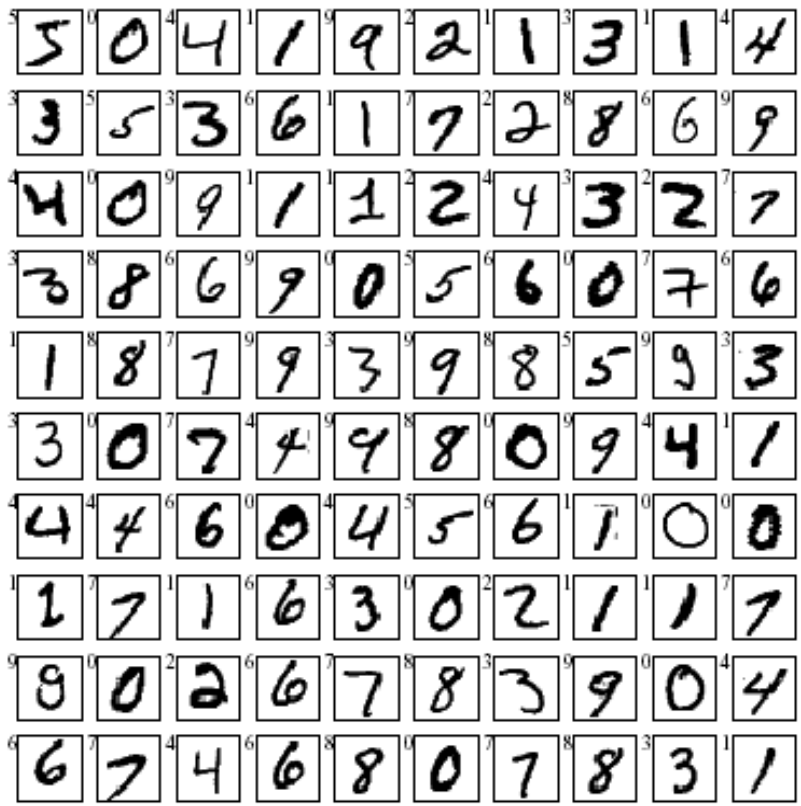
Many Applications

- Handwritten Letter/Digit recognition
- Face/Object detection in natural scenes
- Brain-Computer Interfacing
- Gene Finding
- Drug Discovery
- Intrusion Detection Systems (unsupervised)
- Document Classification (by topic, spam mails)
- Non-Intrusive Load Monitoring of electric appliances
- Company Fraud Detection (Questionaires)
- Fake Interviewer identification in social studies
- Optimized Disk caching strategies
- Optimal Disk-Spin-Down prediction
- …

MNIST Benchmark

handwritten character benchmark (60000 training & 10000 test examples, 28×28)



SVM with polynomial kernel $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x} \cdot \mathbf{x}')^d$

(considers d-th order correlations of pixels)

MNIST Error Rates

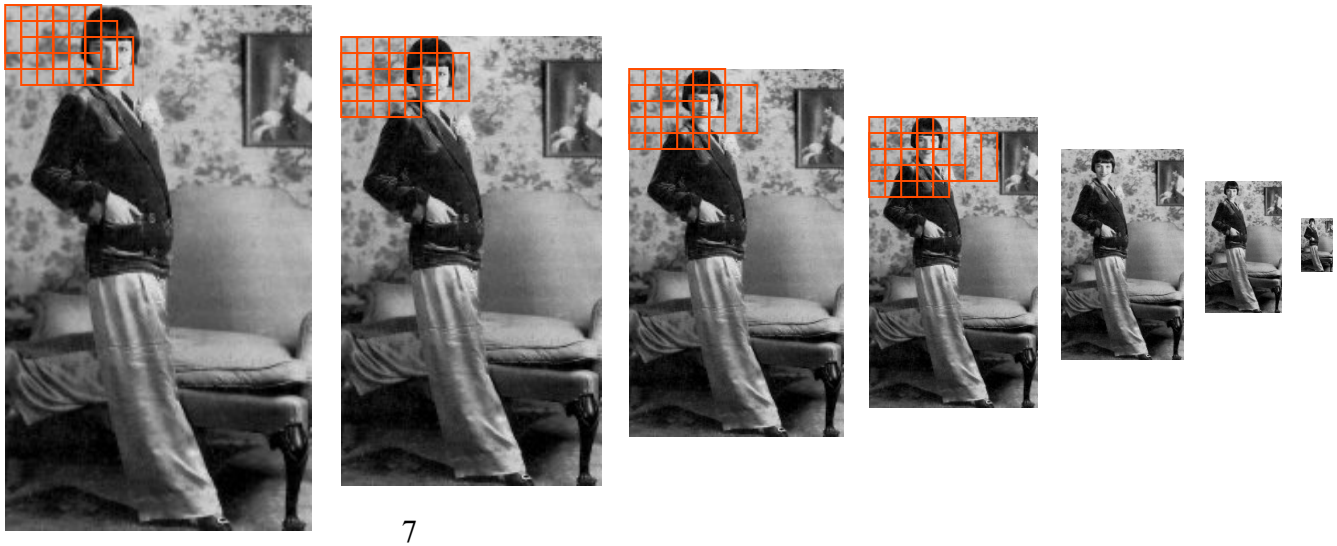
Classifier	test error	reference
linear classifier	8.4%	*Bottou et al. (1994)*
3-nearest-neighbour	2.4%	*Bottou et al. (1994)*
SVM	1.4%	*Burges and Schölkopf (1997)*
Tangent distance	1.1%	*Simard et al. (1993)*
LeNet4	1.1%	*LeCun et al. (1998)*
Boosted LeNet4	0.7%	*LeCun et al. (1998)*
Translation invariant SVM	0.56%	*DeCoste and Schölkopf (2002)*

Face Detection

1.

→ Classifier → face / non-face

2. Search



$$\sum_{l=1}^{7} 600 \cdot 450 \cdot 0.7^{2(l-1)}$$

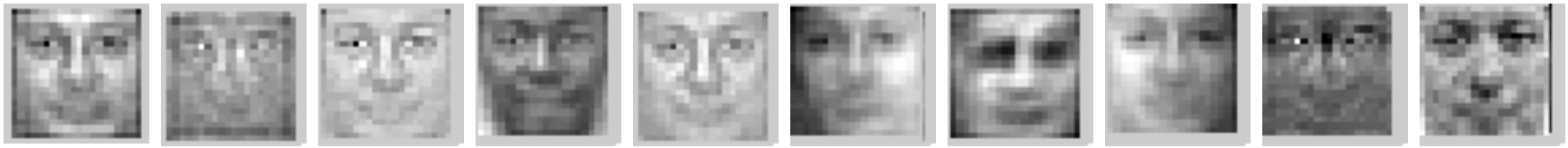
$\Rightarrow$ 525,820 patches

Fast Face Detection

Note: for “easy” patches, a quick and inaccurate classification is sufficient.

Method: sequential approximation of the classifier in a Hilbert space

Result: a set of face detection filters



Romdhani, Blake, Schölkopf, & Torr, 2001

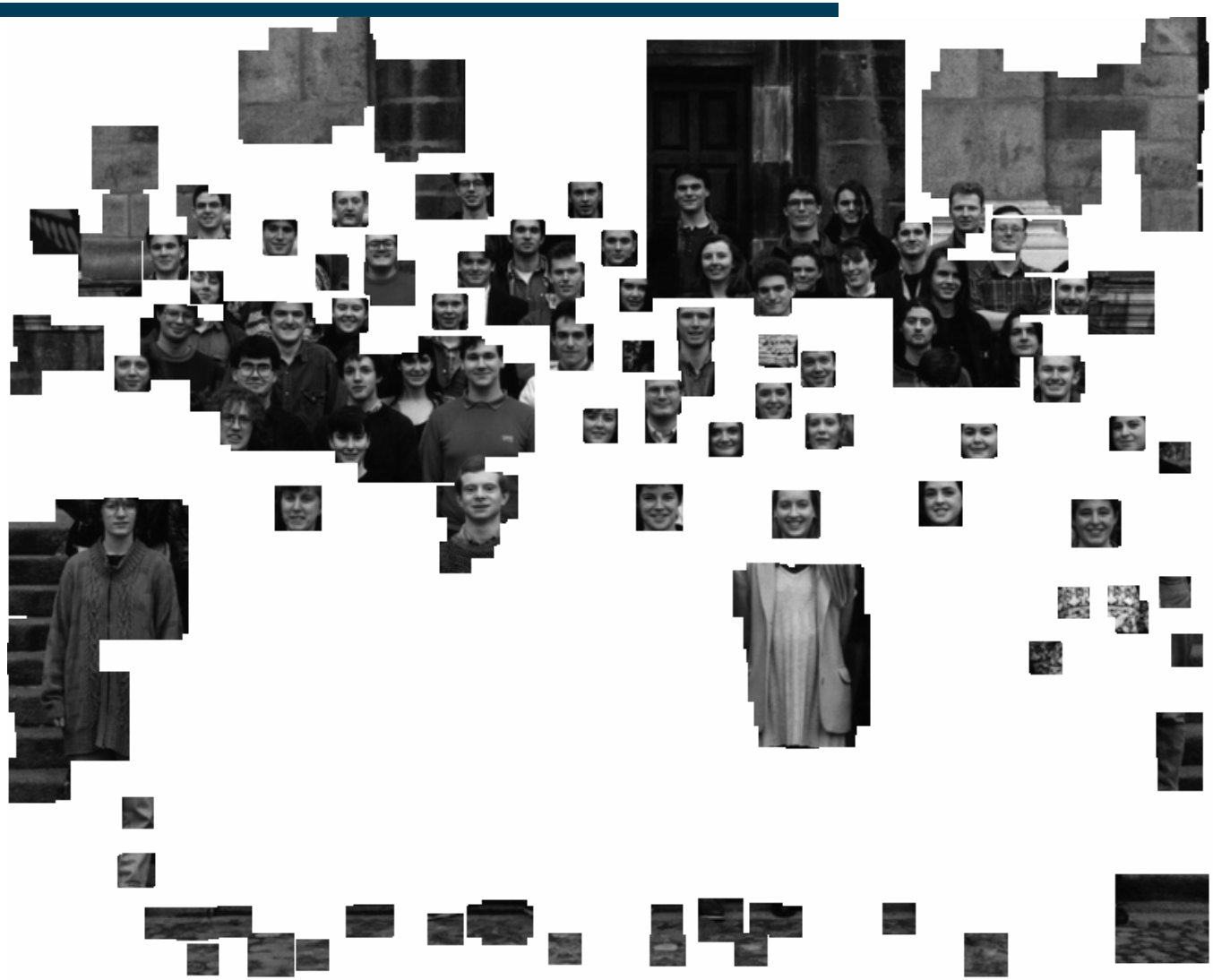
Example: 1280x1024 Image

1 Filter, 19.8% patches left

Example: 1280x1024 Image

10 Filters, 0.74% Patches left

Example: 1280x1024 Image

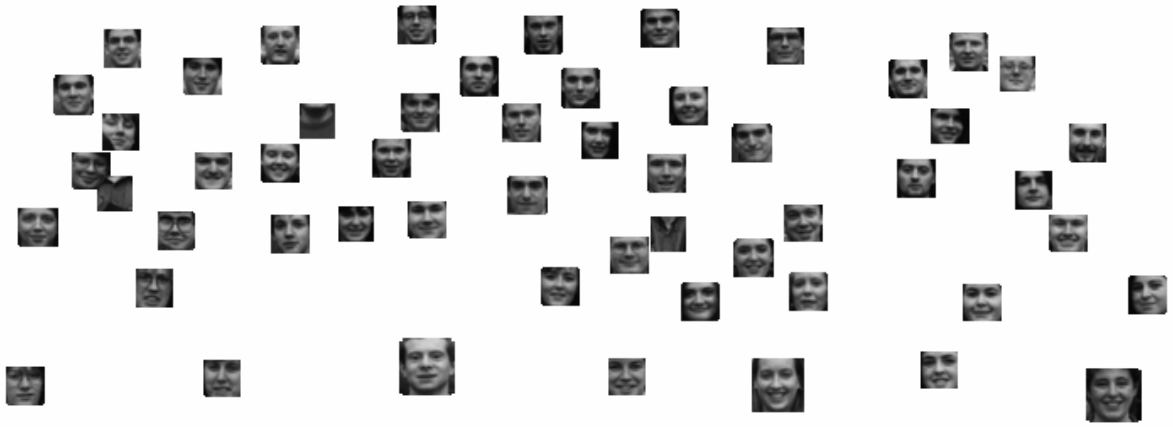


20 Filters, 0.06% Patches left

Example: 1280x1024 Image

30 Filters, 0.01% Patches left

Example: 1280x1024 Image



70 Filters, 0.007 % patches left

Single Trial Analysis of EEG:towards BCI

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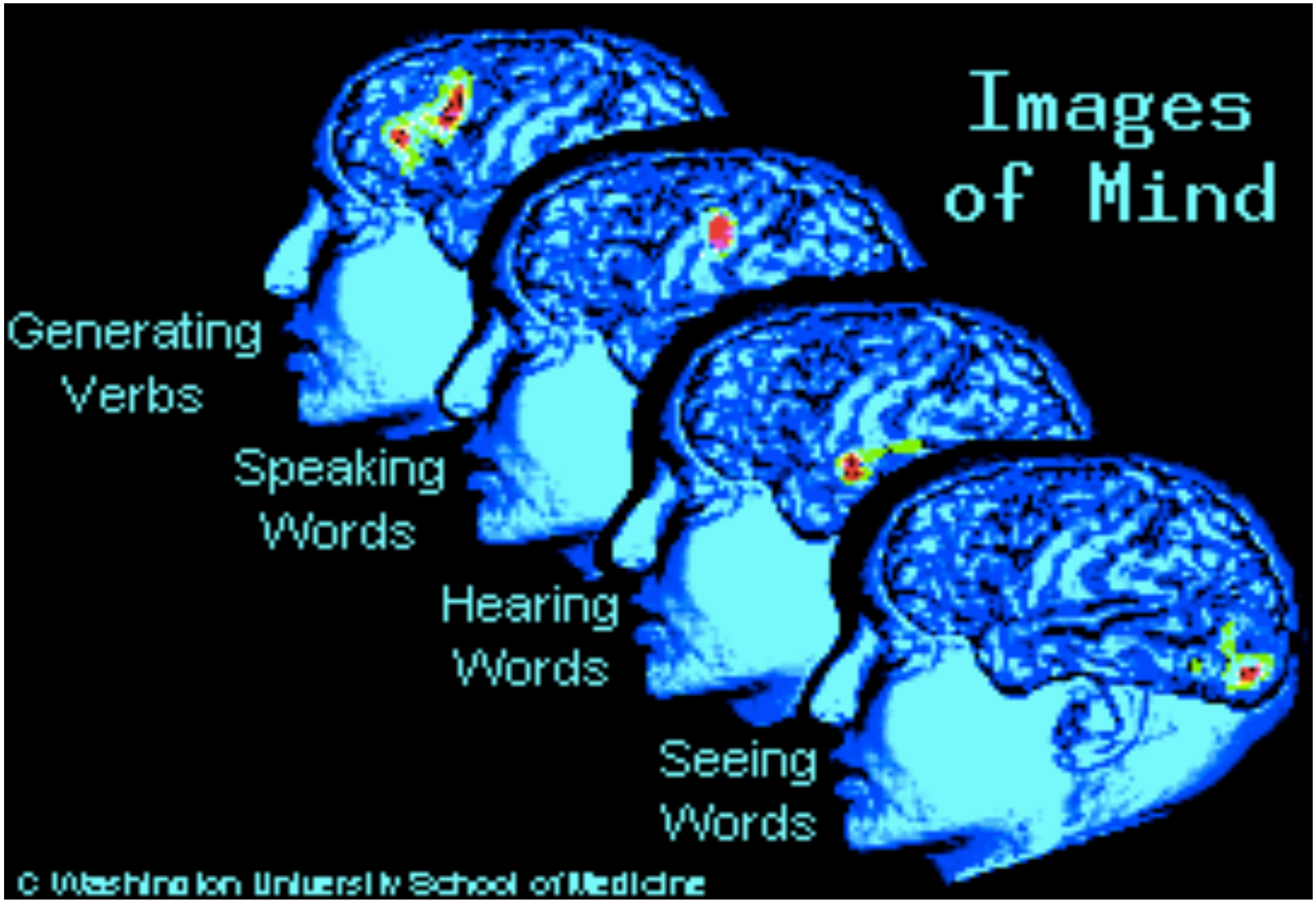
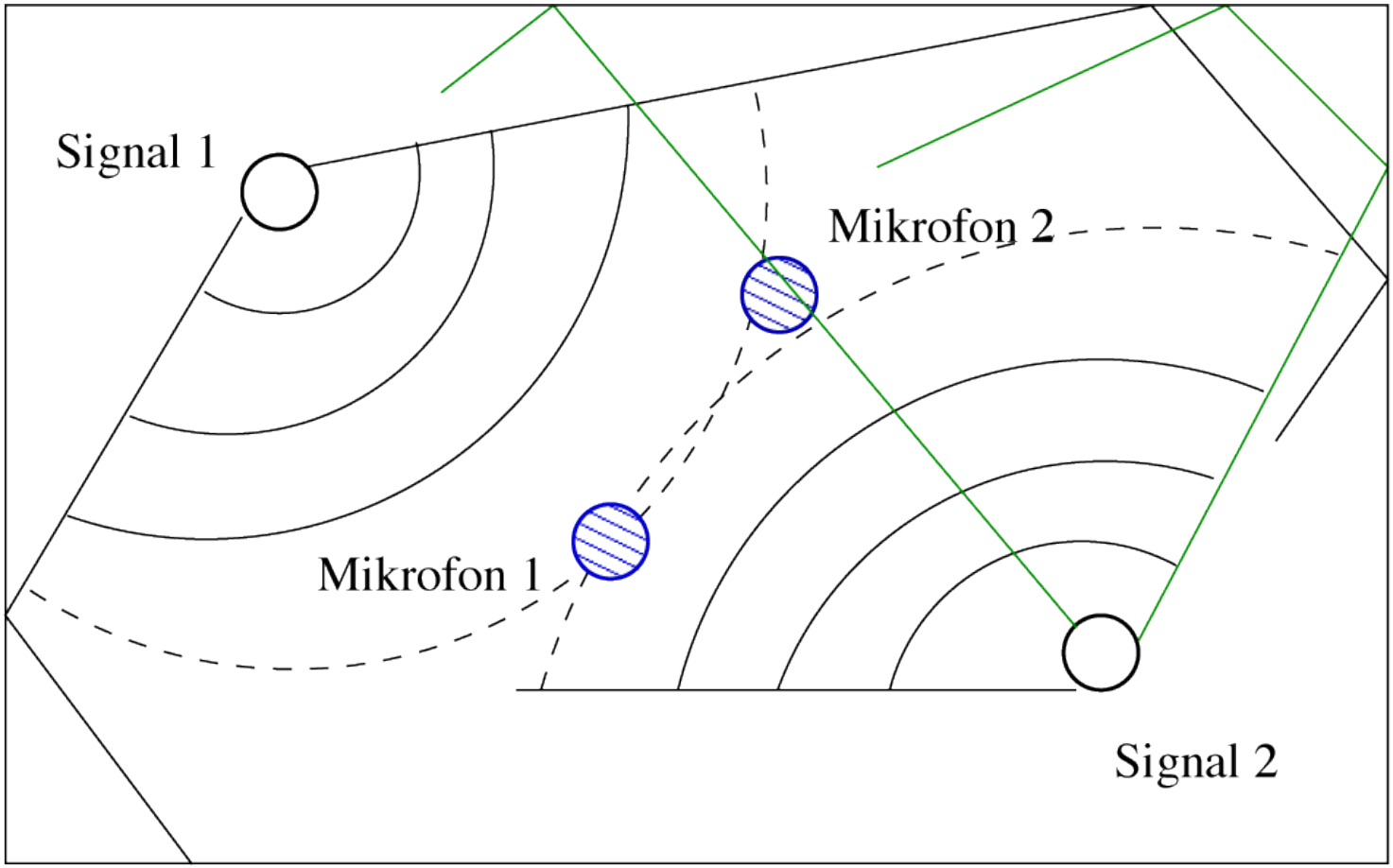
Cerebral Cocktail Party Problem



The Cocktail Party Problem



How to decompose **superimposed** signals?

Analogous Signal Processing problem as for cocktail party problem

The Cocktail Party Problem

- input: 3 mixed signals
- algorithm: enforce *independence* (“independent component analysis”) via temporal de-correlation

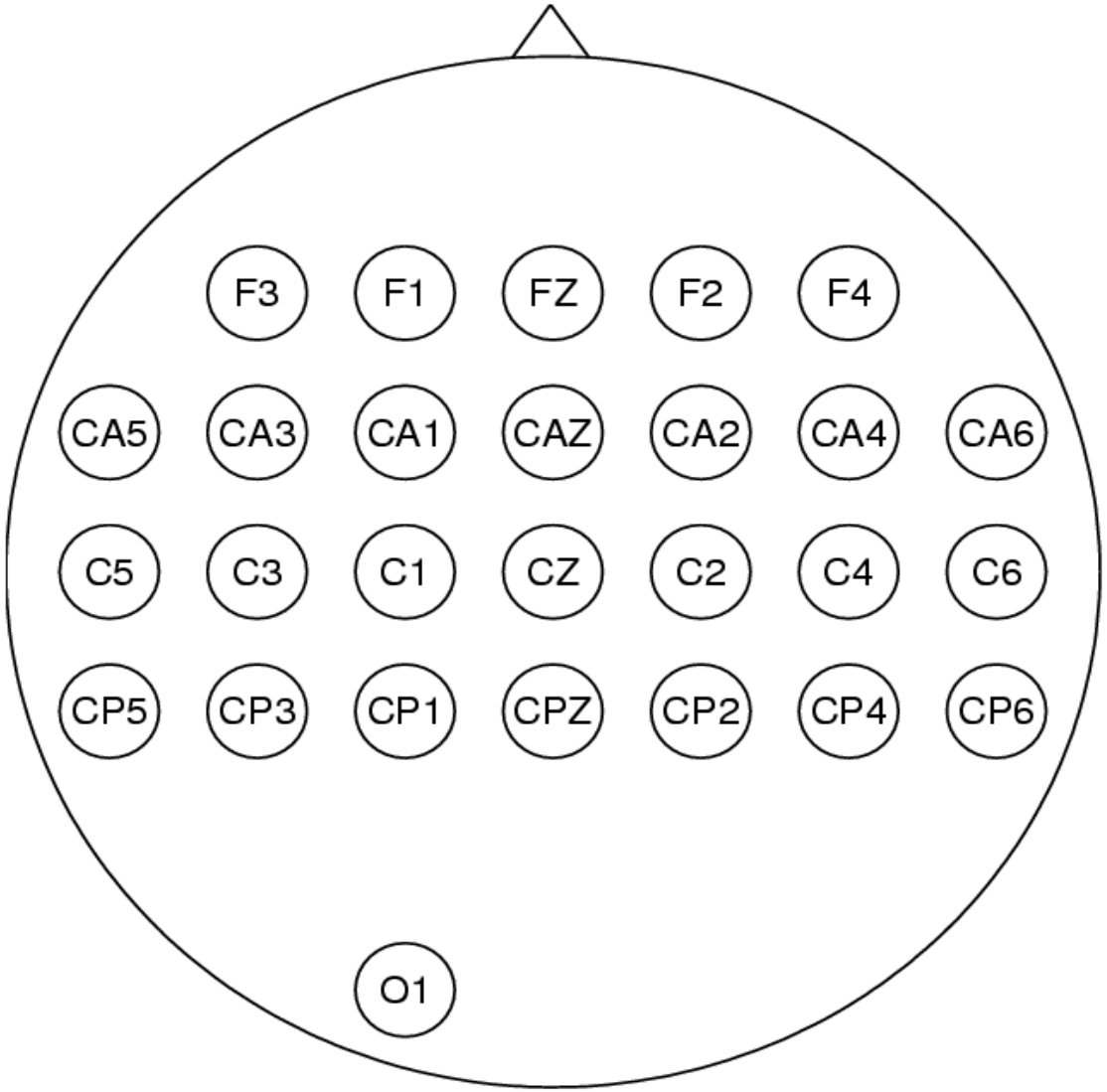
- output: 3 separated signals

"Imagine that you are on the edge of a lake and a friend challenges you to play a game. The game is this: Your friend digs two narrow channels up from the side of the lake […]. Halfway up each one, your friend stretches a handkerchief and fastens it to the sides of the channel. As waves reach the side of the lake they travel up the channels and cause the two handkerchiefs to go into motion. You are allowed to look only at the handkerchiefs and from their motions to answer a series of questions: How many boats are there on the lake and where are they? Which is the most powerful one? Which one is closer? Is the wind blowing?” (**Auditory Scene Analysis**, *A. Bregman*)

(Demo: Andreas Ziehe, Fraunhofer FIRST, Berlin)

Minimal Electrode Configuration

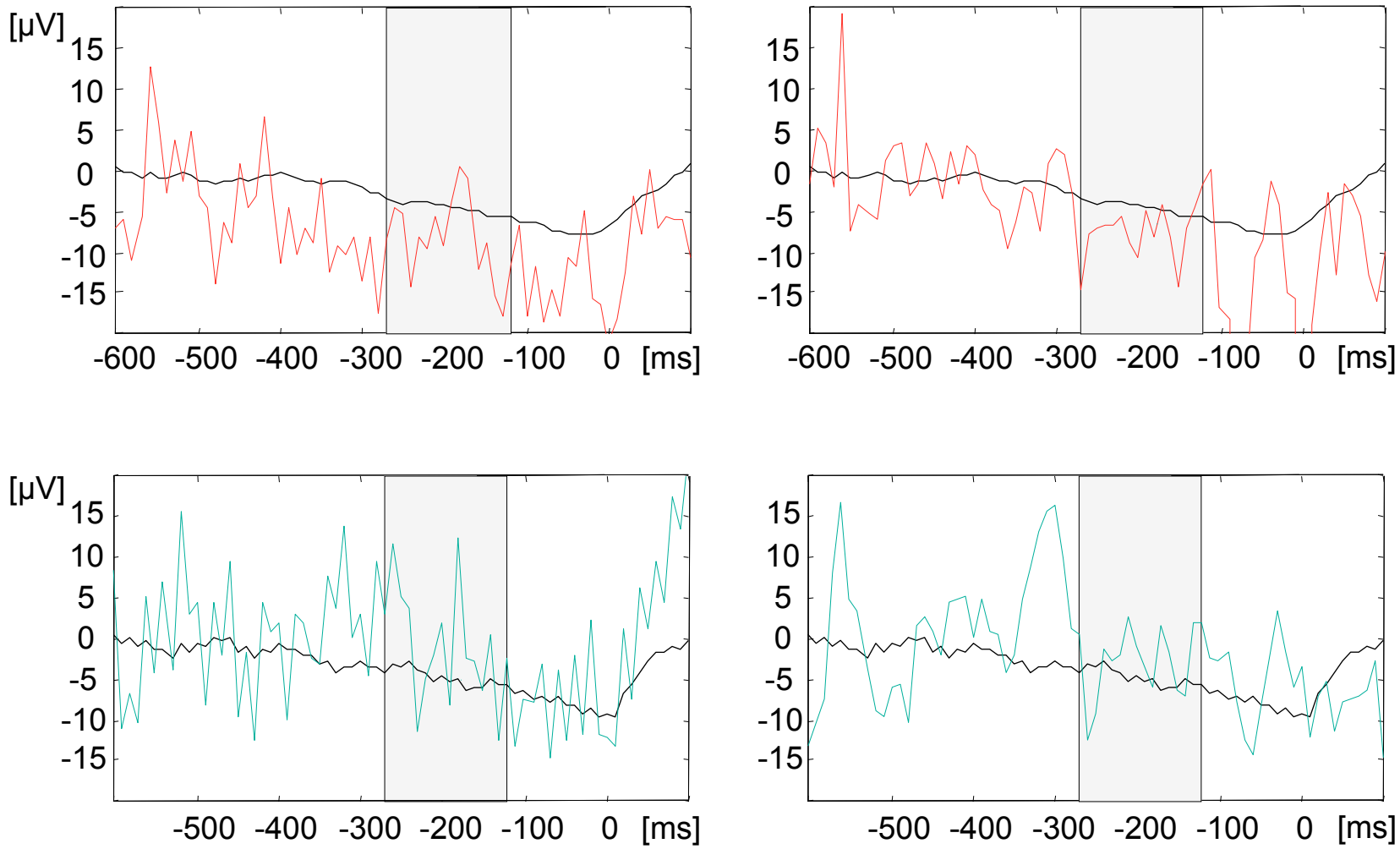
- coverage: bilateral primary sensorimotor cortices
- 27 scalp electrodes
- reference: nose
- bandpass: 0.05 Hz - 200 Hz
- ADC 1 kHz
- downsampling to 100 Hz
- EMG (forearms bilaterally): m. flexor digitorum
- EOG
- event channel: keystroke timing (ms precision)



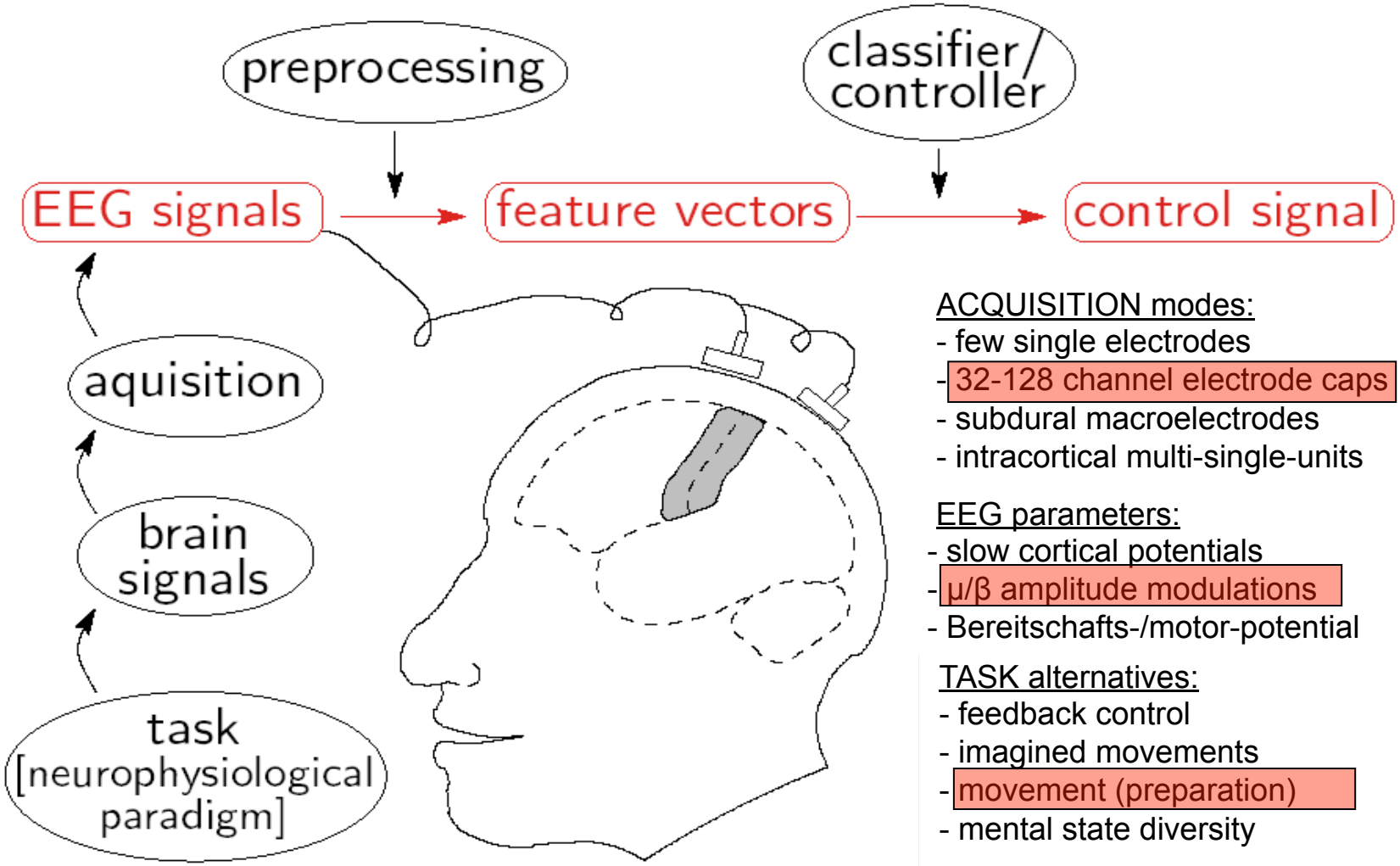
Single Trial vs. Averaging

LEFT hand (ch. C4)

RIGHT hand (ch. C3)



BCI Setup



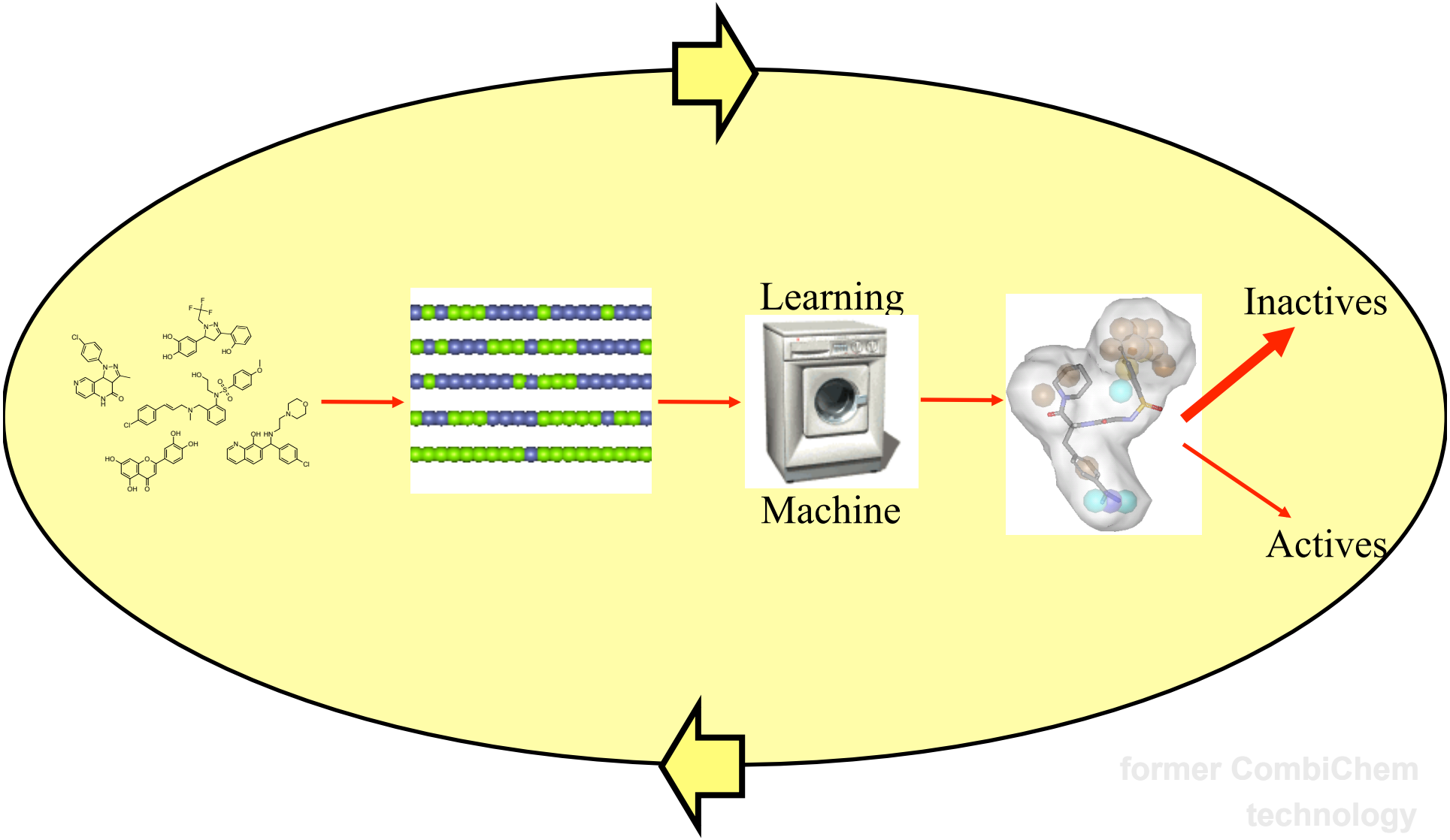
ACQUISITION modes:
- few single electrodes
- 32-128 channel electrode caps
- subdural macroelectrodes
- intracortical multi-single-units

EEG parameters:
- slow cortical potentials
- μ/β amplitude modulations
- Bereitschafts-/motor-potential

TASK alternatives:
- feedback control
- imagined movements
- movement (preparation)
- mental state diversity

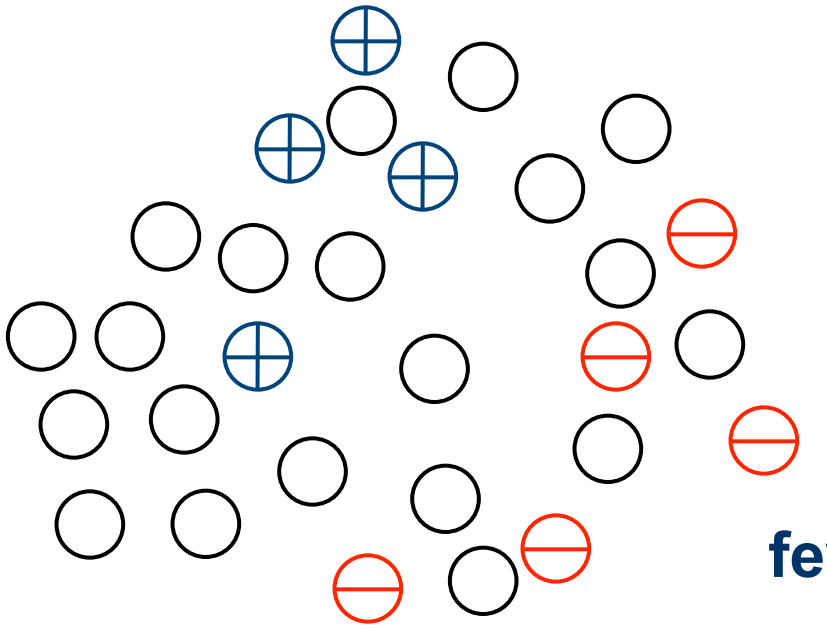
5
NIPS 2003

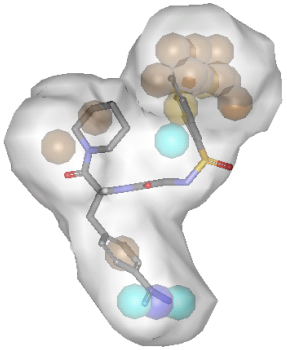
The Drug Design Cycle



former CombiChem technology

Three types of Compounds/Points



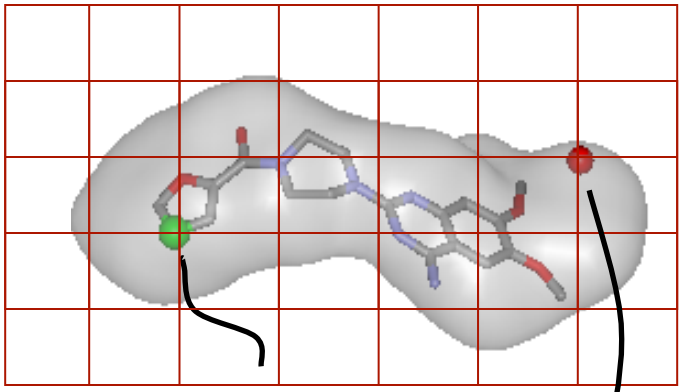


few ⊕ actives

more ⊖ inactives

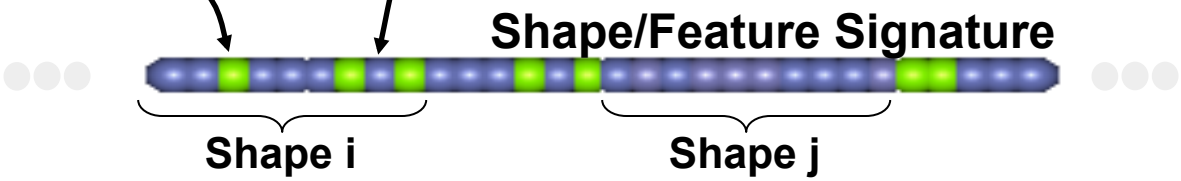
plenty ○ untested

Shape/Feature Descriptor



bit number
254230

bit = { Shape, Feature type, Feature location }



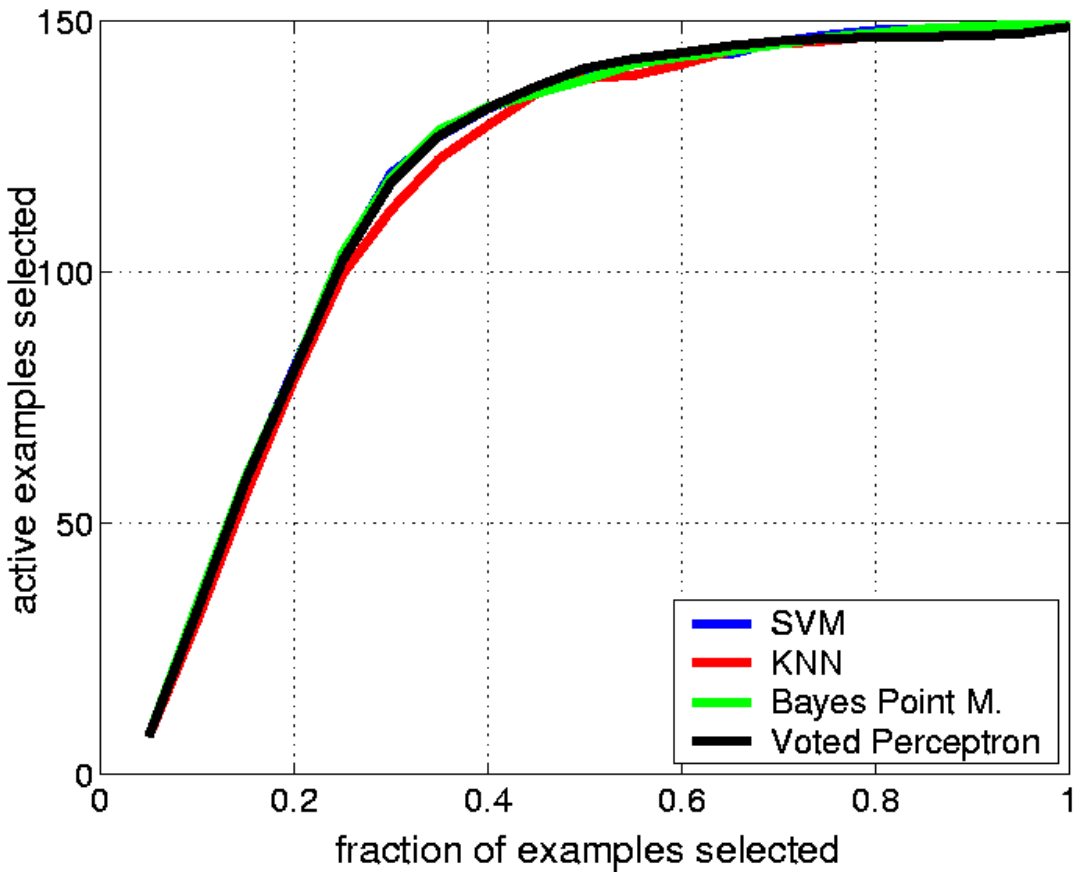
~10^5 bits

S. Putta, *A Novel Shape/Feature Descriptor*, 2001

Maximizing the Number of Hits

Total number of active examples selected after each batch

On Thrombin dataset



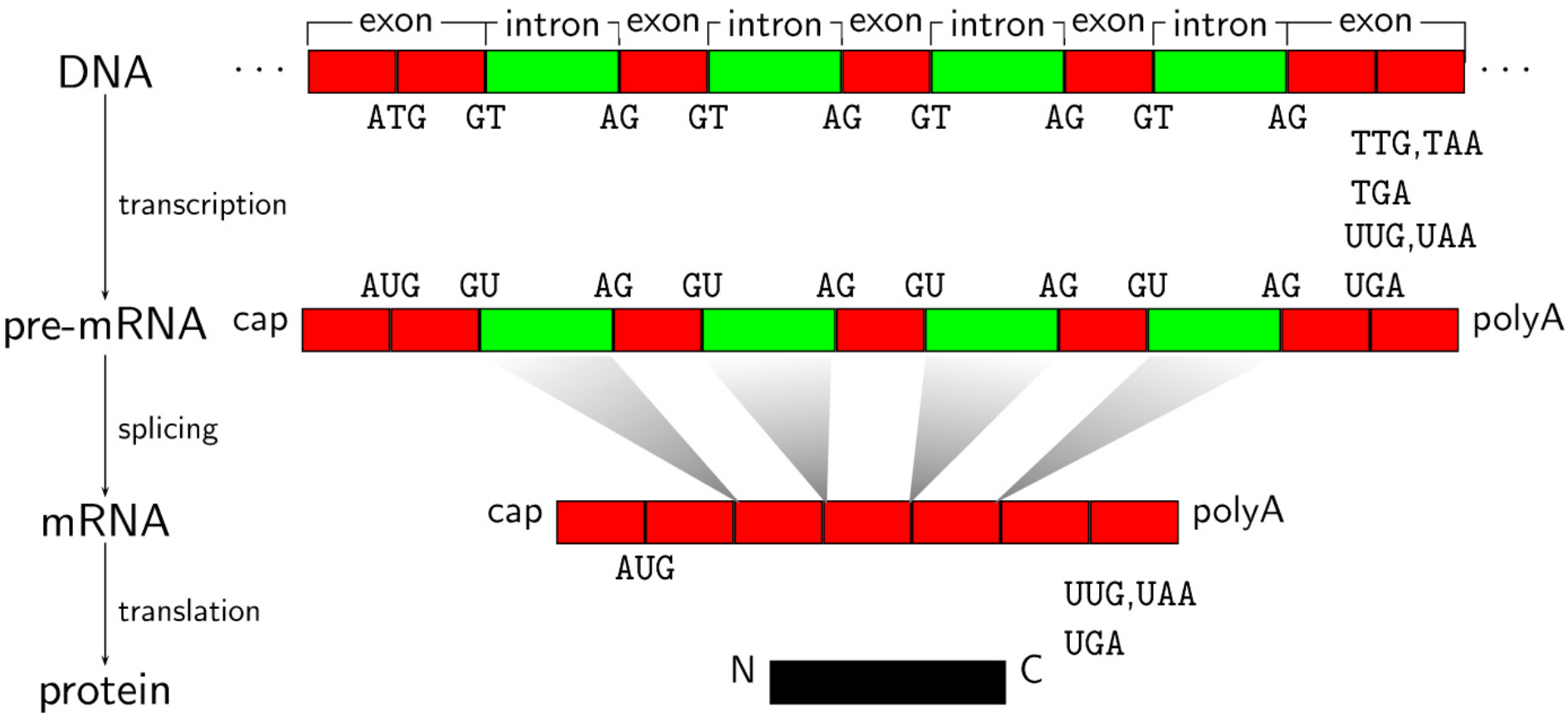
***Largest* Selection Strategy**

Finding Genes on Genomic DNA

Splice Sites: on the boundary

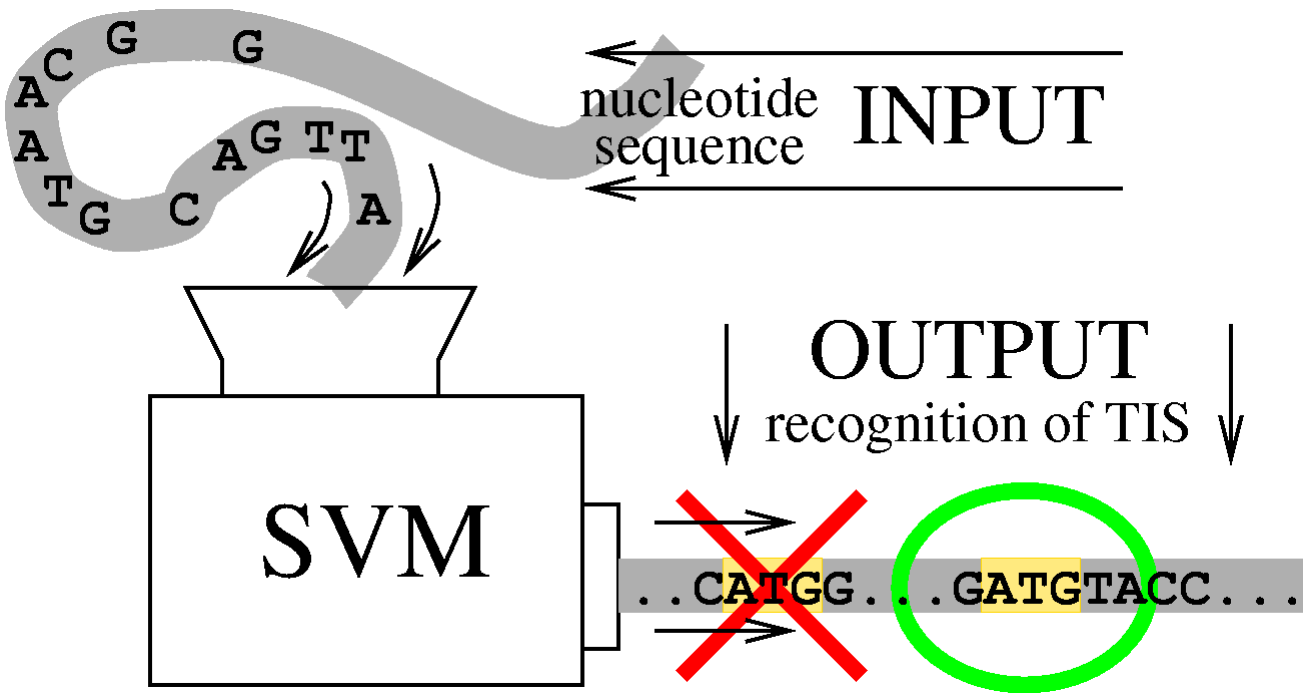
- **Exons (may code for protein)**
- **Introns (noncoding)**

Coding region starts with Translation Initiation Site (TIS: "ATG")



Application: TIS Finding

Engineering Support Vector Machine (SVM) Kernels That Recognize Translation Initiation Sites (TIS)



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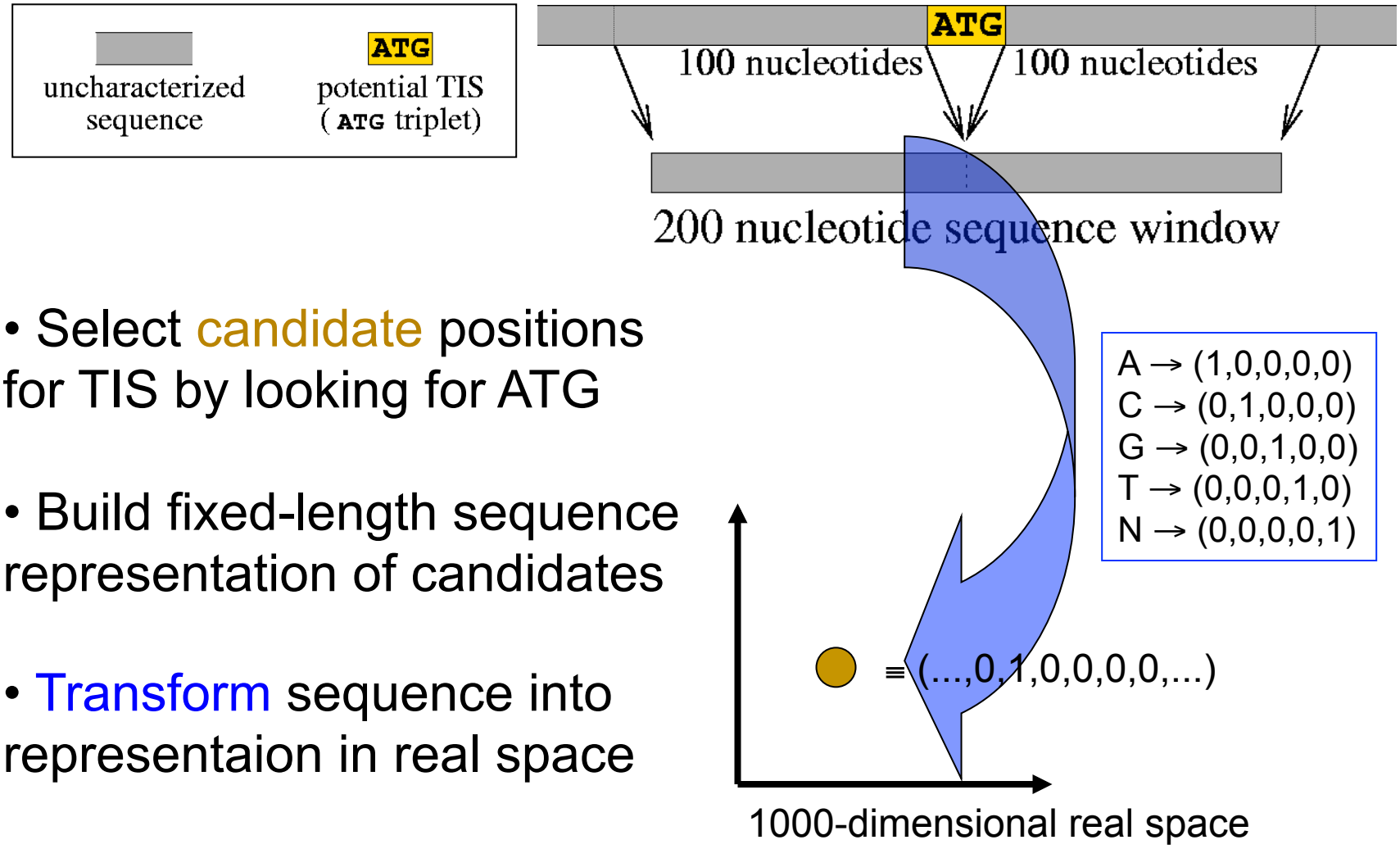
TIS Finding: Classification Problem



- Select candidate positions for TIS by looking for ATG
- Build fixed-length sequence representation of candidates
- Transform sequence into representaion in real space

2-class Splice Site Detection

Window of 150nt

CT...GTAGAG TGTA..GAAGCT AG GAGCGC..ACCGT ACGCGT...GA

around known splice sites

Positive examples: fixed window around a true splice site
Negative examples: generated by shifting the window

```
AAACAAATAAGTAACTAATCTTTTAGGAAGAACGTTTCAACCATTTTGAG
AAGATTAAAAAAAAACAAATTTTTAGCATTACAGATATAATAATCTAATT
CACTCCCCAAATCAACGATATTTTAGTTCACTAACACATCCGTCTGTGCC
TTAATTTCACTTCCACATACTTCCAGATCATCAATCTCCAAAACCAACAC
```

Design of new Support Vector Kernel

$k(s_1,s_2) = w_7 + w_1 + w_2 + w_2 + w_3$

```
S1 → AGTCAGATAGAGGACATCAGTAGACAGATTAAA →
     |||||||      ||   ||       |||
S2 → TTATAGATAGACAAAGACATCAGTAGACTTATT →
```

Some Remarks

- Computational Challenges
  - Algorithms can work with 100M's of examples (need $\mathcal{O}(N^2)$ - $\mathcal{O}(N^3)$ operations
  - Usually model parameters to be tuned (cross-validation ⇒ computationally expensive)
  - Need computer clusters and Job scheduling systems (pbs, gridengine)
  - Use Python/MATLAB/R/…

- Machine learning is an exciting research area …
- … involving Computer Science, Statistics & Mathematics
- … with…
  - **a large number of present and future applications (in all situations where data is available, but explicit knowledge is scarce)…**
  - **an elegant underlying theory…**
  - **and an abundance of questions to study.**

Thanks for Your Attention! (Part 1)

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