SAPIENZA
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AI AND MACHINE LEARNING
A QUICK INTRODUCTION …

Methods in experimental particle physics
Roma 29.5.2020
S. Giagu

REFERENCES AND FURTHER READING …

- Machine Learning and Deep Learning:
  - Stat. Pattern Recognition: A. Webb, (3rd ed.), J.Wiley&Sons
  - C.M. Bishop: Pattern Recognition and Machine Learning, Springer
  - Decision Forests for Computer Visions and Medical Image Analysis: A.Criminisi, J.Shotton, Springer
  - Deep Learning: I.Goodfellow, Y.Bengio, A.Courville, The MIT Press

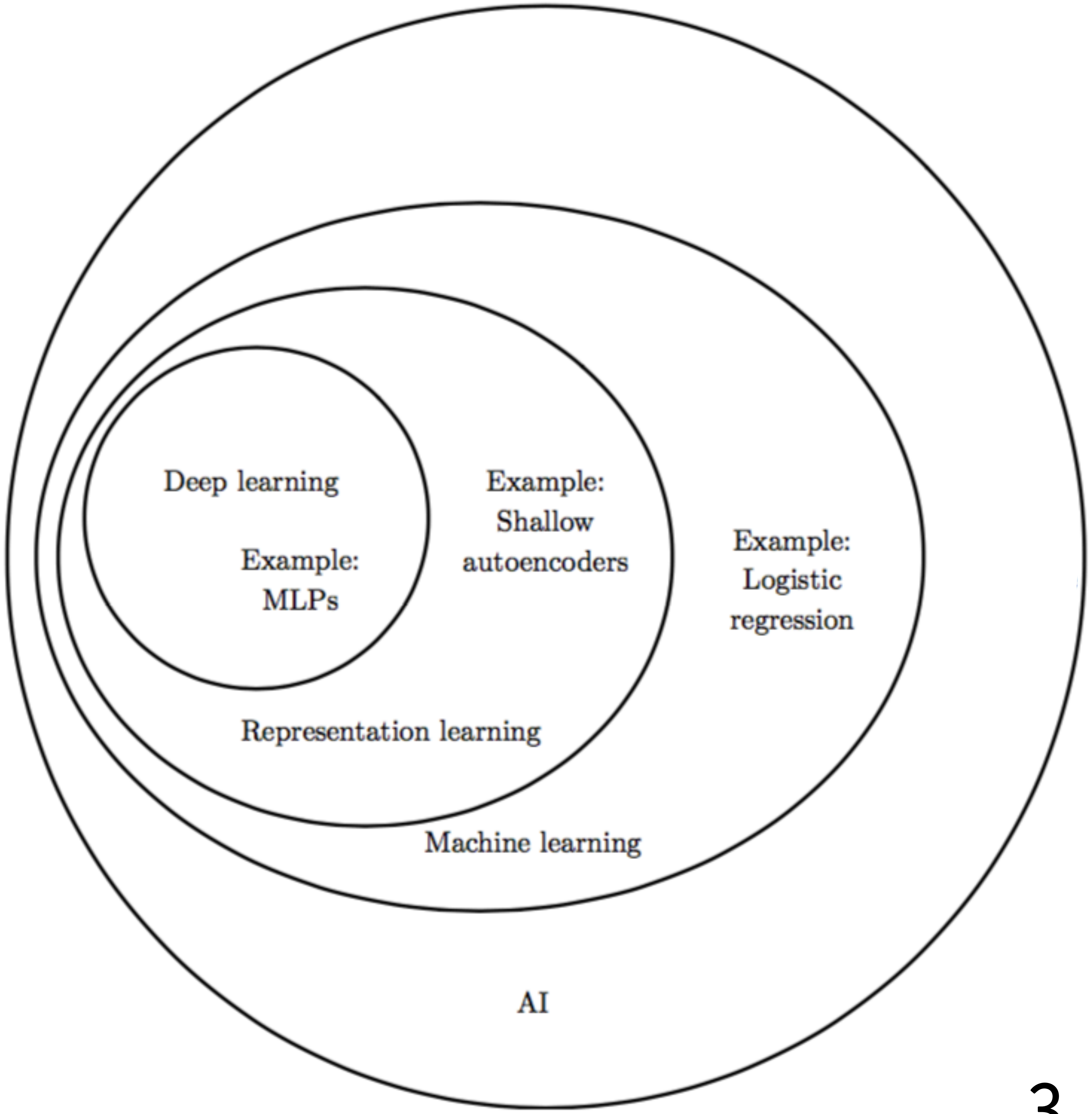
- Artificial Intelligence (introductive):
  - Artificial Intelligence: A Modern Approach: P.Norvig. (free on web)
  - Life 3.0 – Being Human in the Age of Artificial Intelligence: M. Tegmark
  - Fundamental Algorithms: 1 (Artificial Intelligence for Humans): J.Heaton (more advanced)

- Tools/frameworks:
  - Scikit-learn: https://scikit-learn.org/stable/
  - Keras & TensorFlow:https://www.tensorflow.org
  - PyTorch: https://pytorch.org

INTRODUCTION

- What Machine Learning means?

  - ML is part of a larger research filed called Artificial Intelligence (AI) focused in the attempt to automatize intellectual tasks that are generally performed by humans



AI

- the AI concept and the study and development of ML algorithms used in AI systems started in the early 50', but it is only in the last ~10 years that AI applications are spreading exponentially in the society outside the basic and accademico research field

- This acceleration motivated by three parallel developments:
  - better algorithms (Machine & Deep Learning)
  - higher computing power (GPUs/TPUs/HPCs)
  - ability of the technological and industrial sectors to record and make accessible huge amounts of data/information (grid, clouds)

MACHINE LEARNING

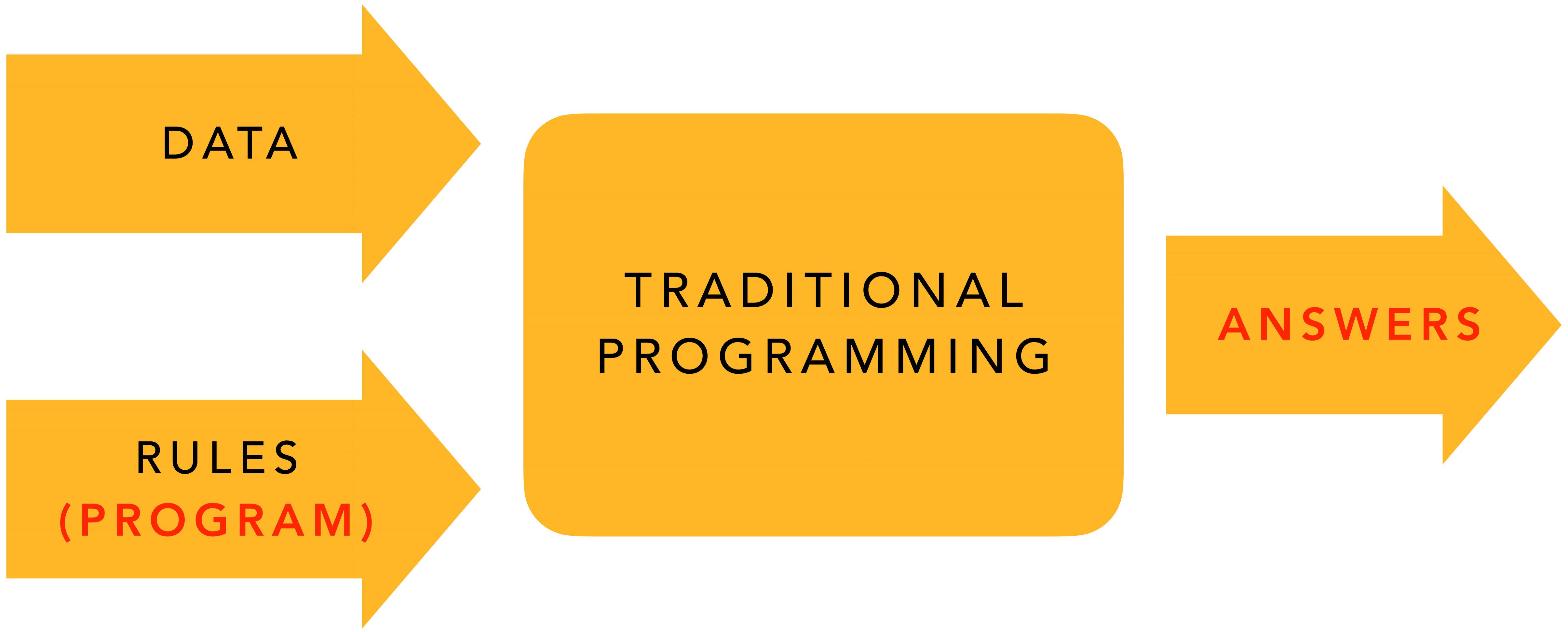
- Original definition (Arthur Samuel, 1959):

  Computational methods (algorithms) able to emulate the typical human, or animal, behaviour of learning based on the experience (i.e. learning from examples), w/o being explicitly programmed

  ML algorithms are meant to solve that class of problems (like image or language recognition) that cannot be simply described with a set of formal mathematical rules (equations) and so too complex to be resolved by a traditional computational algorithm

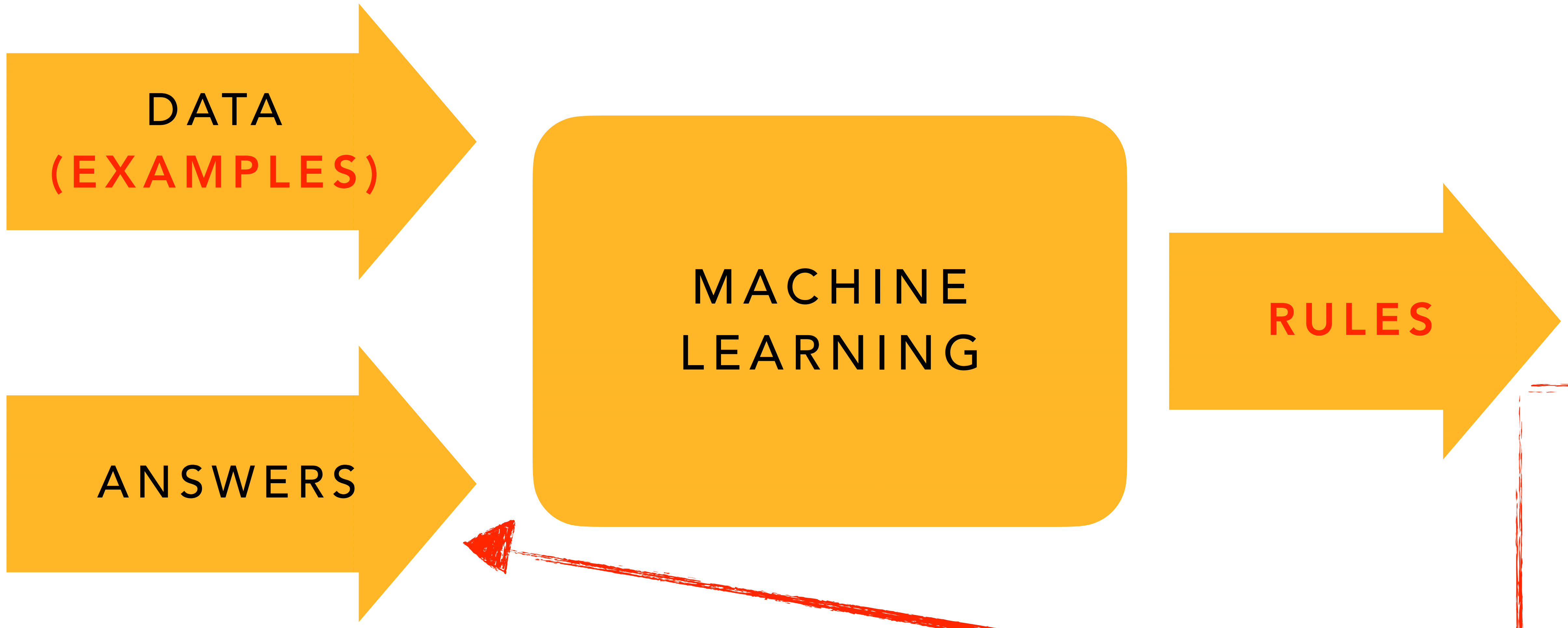
MACHINE LEARNING VS TRADITIONAL COMPUTATION

- Traditional computation (symbolic AI): the programmer (human) design and load a set of rules (program) in the processor together a set of data that are analysed accordingly the set of rules to output an answer to the problem we want to solve



MACHINE LEARNING VS TRADITIONAL COMPUTATION

- ML: the programmer present to the processor both the data set and the set of answers expected for that data set. The algorithm output a set of rules that can then applied to indipendenti datasets to get the original answers



NOTE: answers can be also identified by the algorithm itself inside the training set (unsupevised or self-supervised learning)

a ML system is “trained” not programmed …

- is feed with a set of relevant examples gli vengono presentati un certo numero di esempi significativi
- try to find statistical structures in these examples (we assume these structures exist), that eventually will allow the algorithm to learn the rules needed to learn to perform a certain task

A MODERN DEFINITION (MITCHELL, 1998)

- an algorithm is said to learn from experience (E) with respect to some class of tasks (T) and a performance measure (P), if its performance at tasks in T, as measured by P, improves with experience E

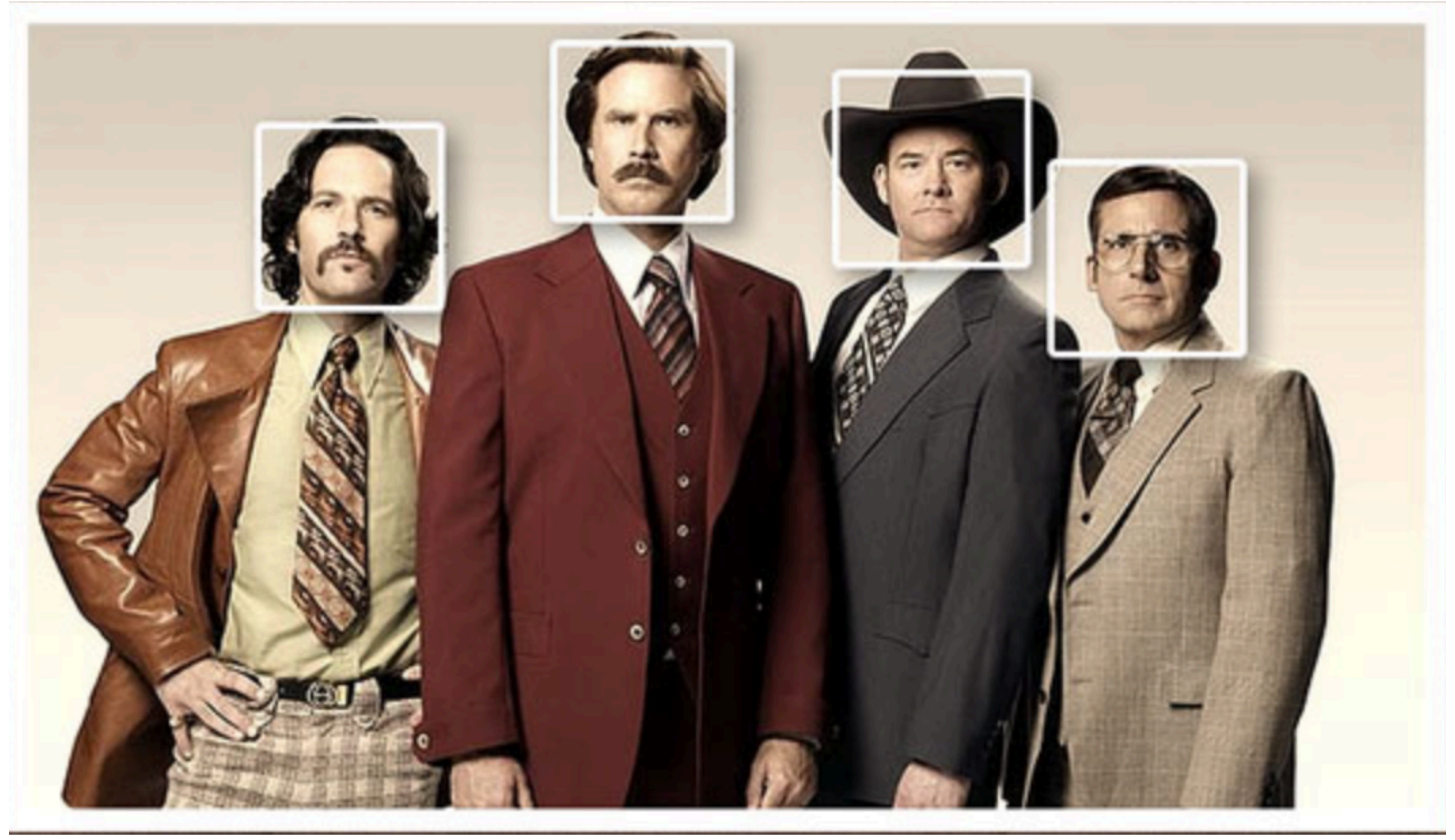
- Task T: are described in terms of how the ML algorithm should process the example E
    - typical ML tasks:
        - classification ($f:R^n \rightarrow \{1,\ldots,k\}$), regression ($f:R^n \rightarrow R^m$), images segmentation, transcription (ex. OCR), conversion of sequences of symbols (automatic translation), anomaly detection, synthesis/sampling (es. generators), de-noising, …

- Example/Experience E:
  - represent the set of empirical information from which the algorithm learn
    - training set (i.e. the data)
    - prior knowledge: invariants, correlations, …

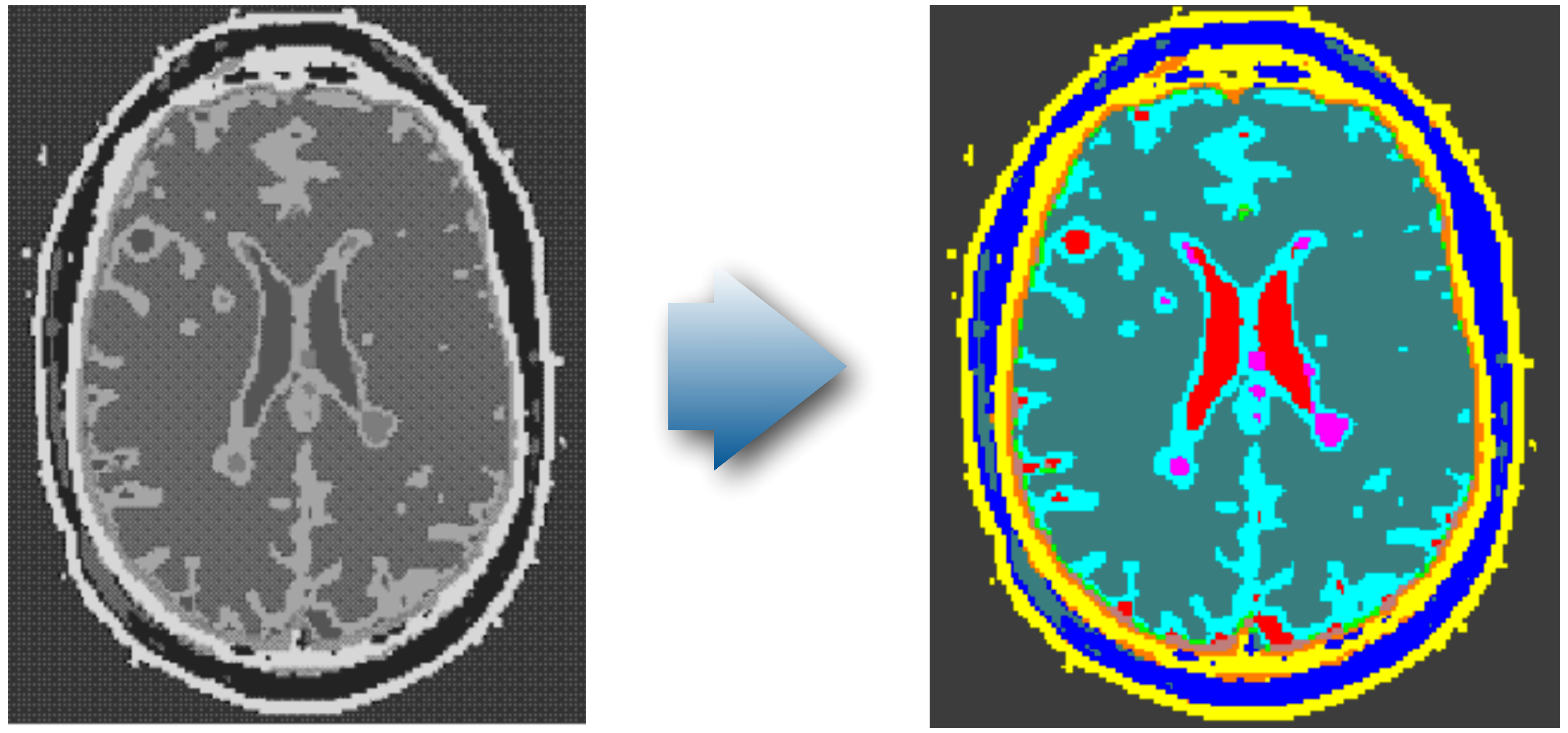
- Performance measure P: to evaluate the abilities of a machine learning algorithm, we must design a quantitative measure of its performance. Usually this performance measure P is specific to the task T being carried out by the system
  - accuracy (fraction fo examples for which the algorithm produce the correct output), error rate, statistical costs, ROC, AUC, …
  - must be always evaluated in a statistically independent data set (test sample)

AI/ML TASK EXAMPLES

Face/Object Detection:
- static: ex. facebook photos
- real time: cameras, autonomous driving systems
- experience: portion of images
- task: face or not-face



Medical Image Detection e Segmentation:
- experience: images (list of pixels)
- task: identify different biological tissues, disomogeneities ...

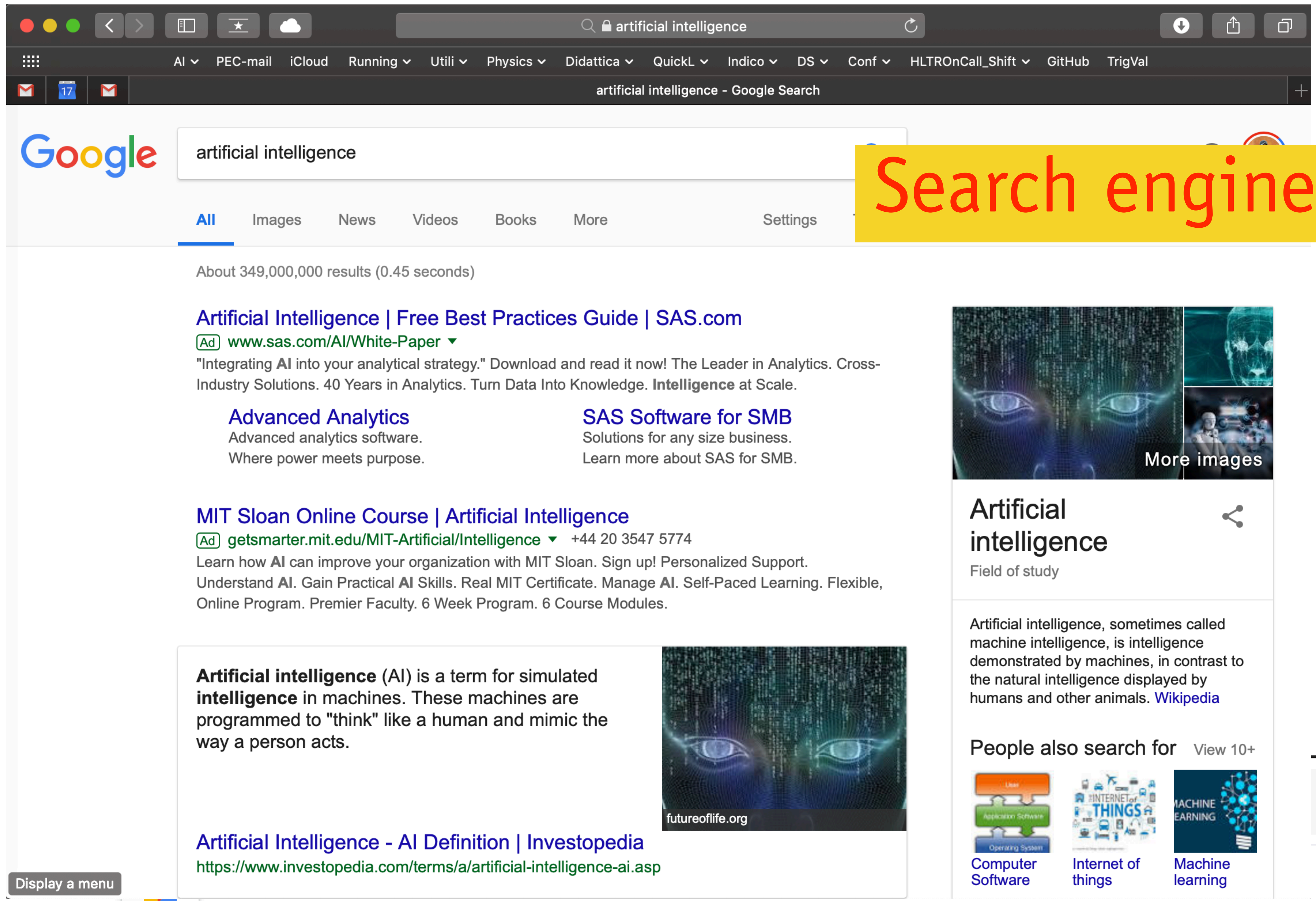


Voice recognition:
- experience: acoustical signals
- task: identify phonemes

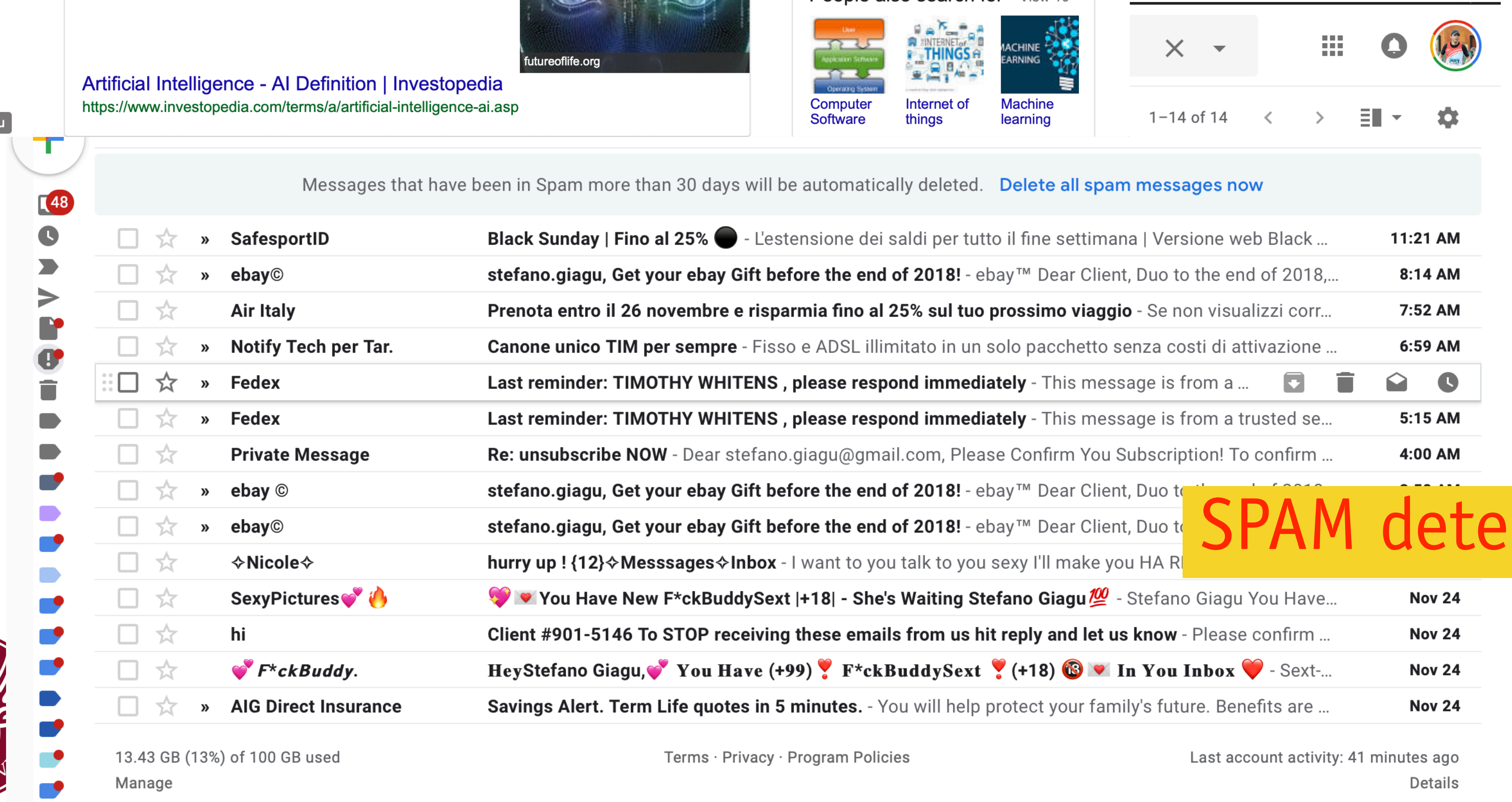
ma-chin-le-ar-nin-g

AI/ML TASK EXAMPLES

Search engines



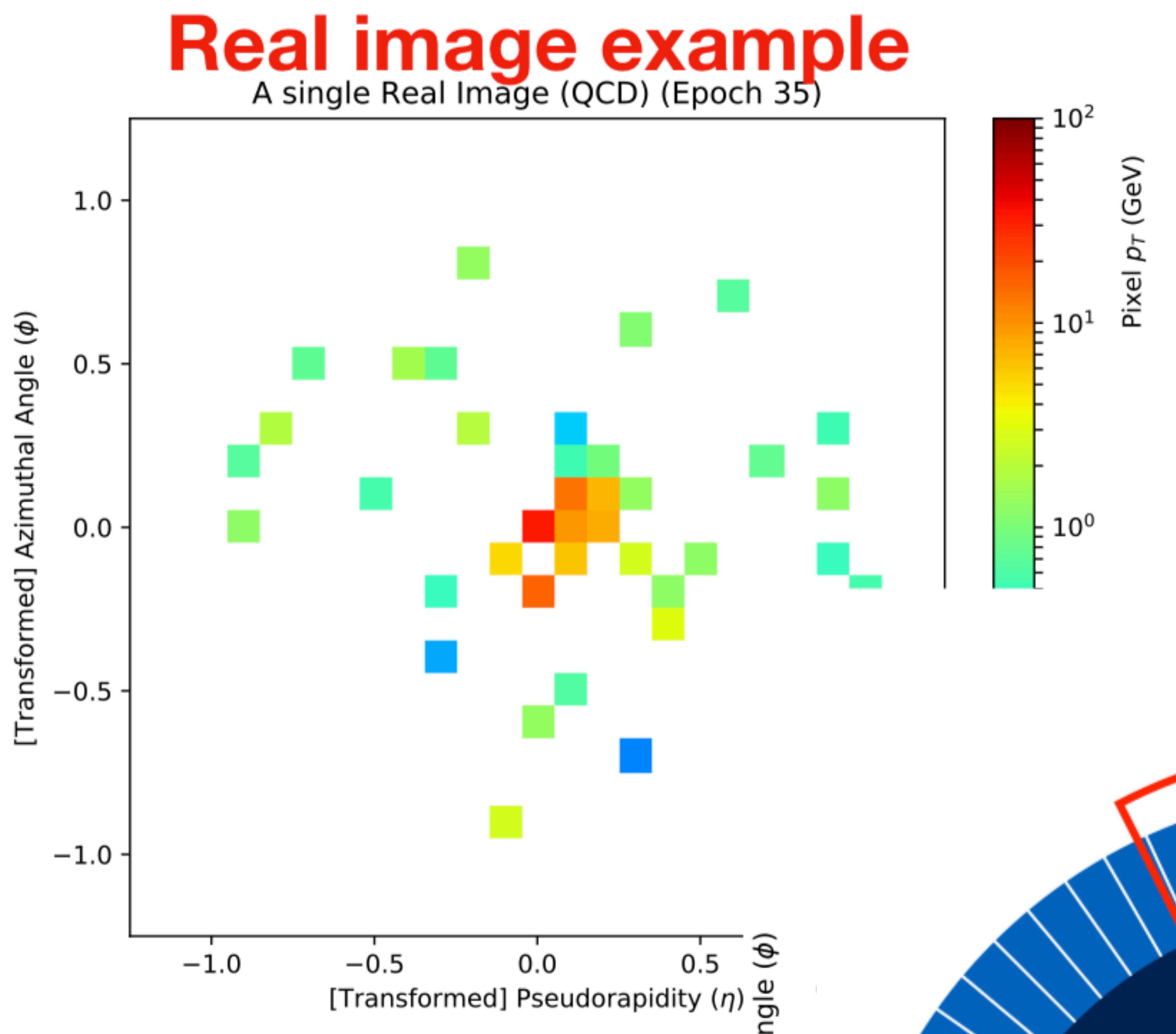
Autonomous drive

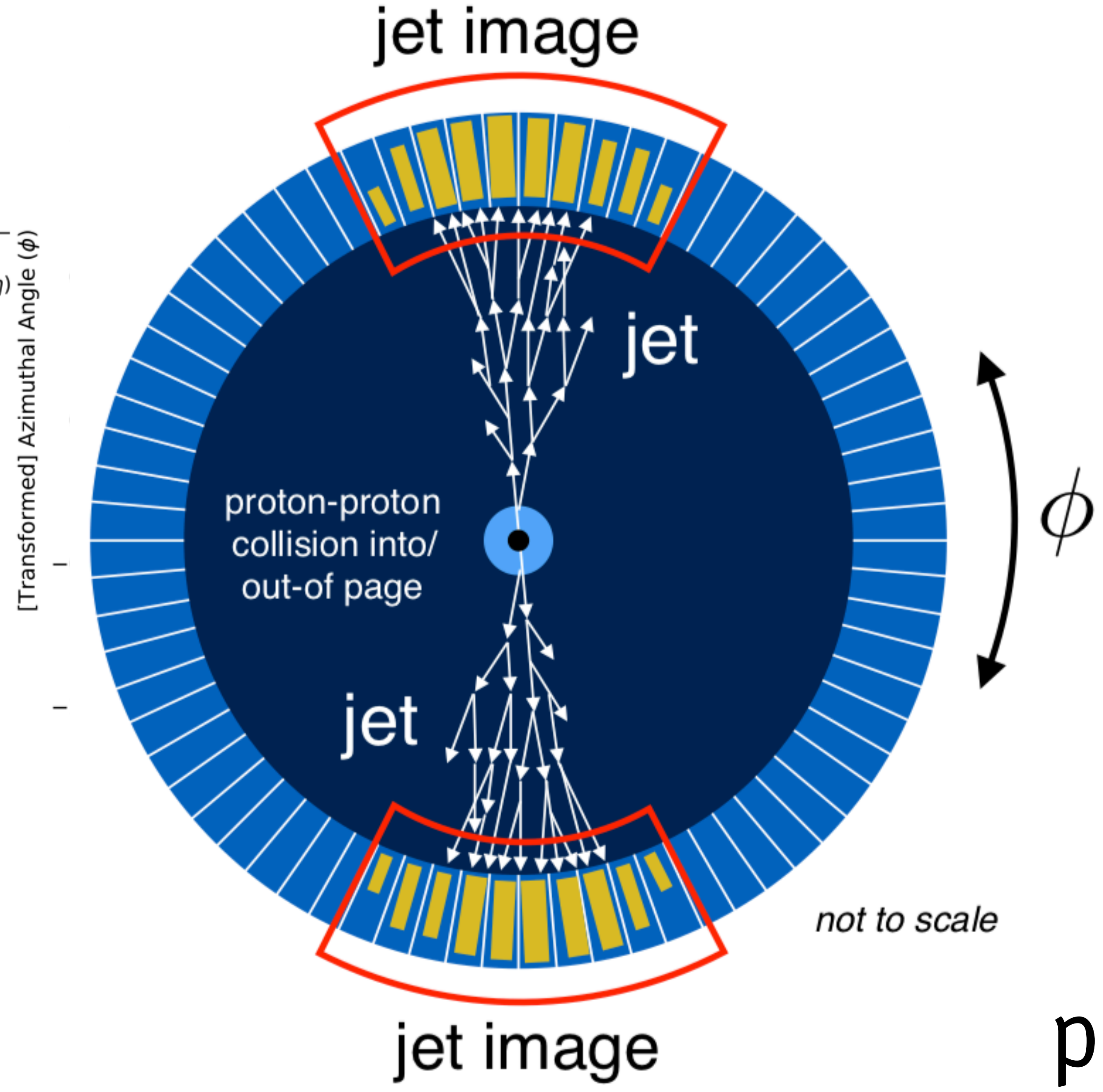


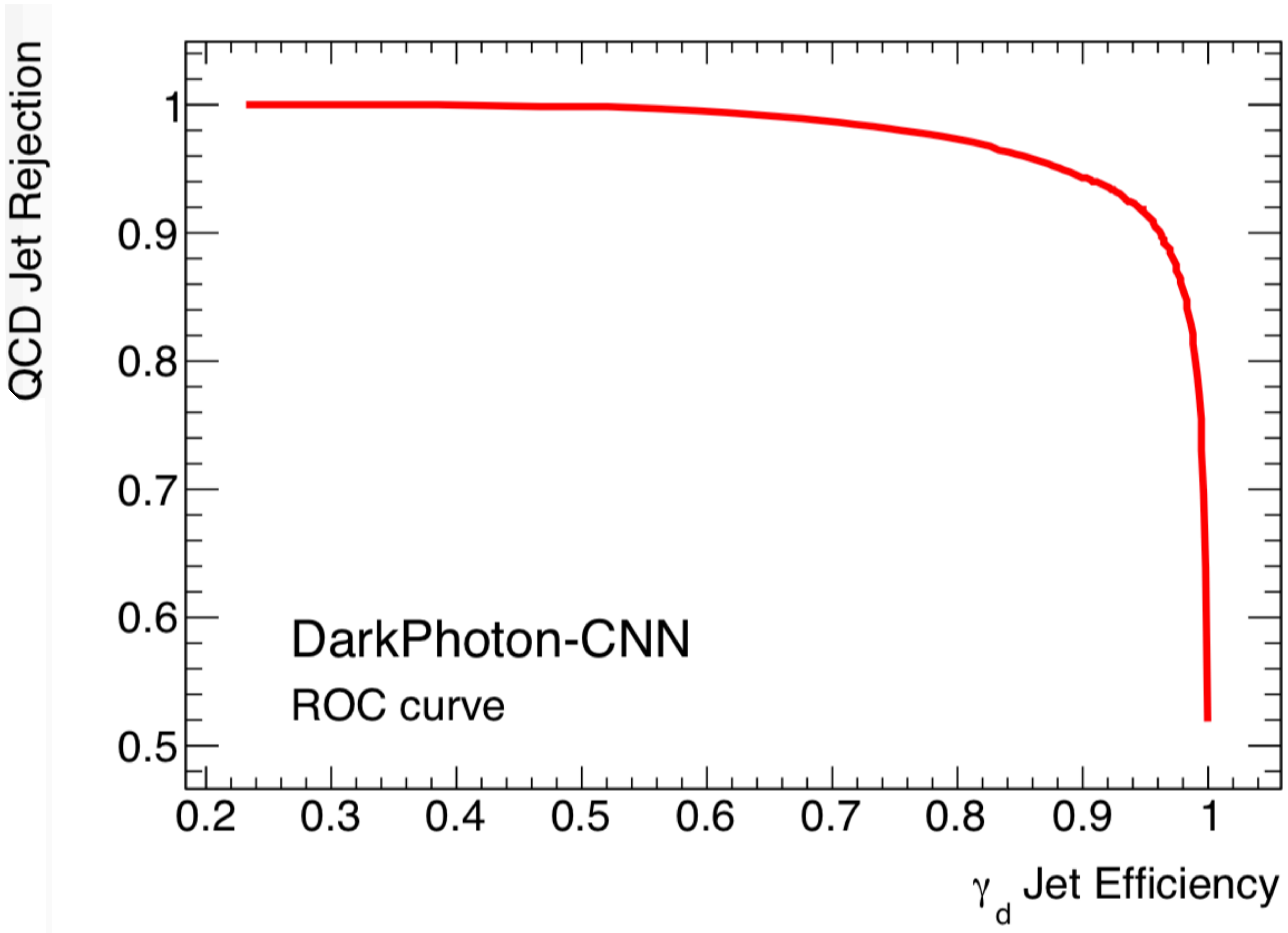
SPAM detection

Autonomous Drones

EXAMPLE OF A TASK IN HEP: CONVNET TO CLASSIFY HADRONIC JETS





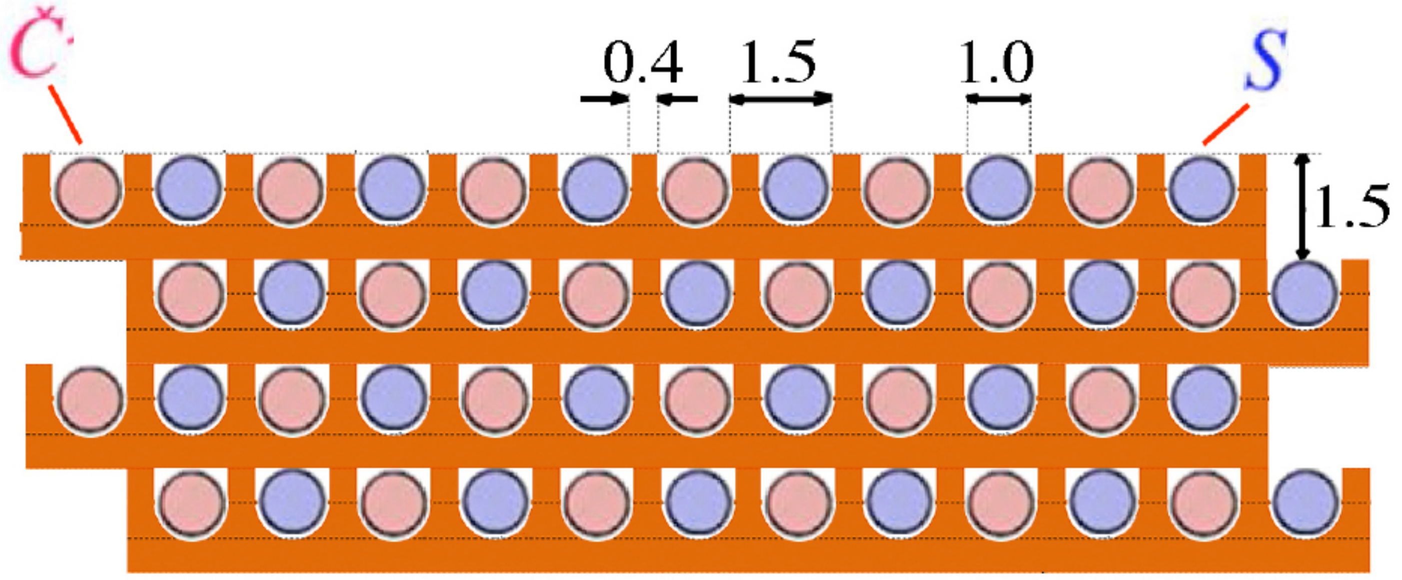


pp → qq → 2 jet

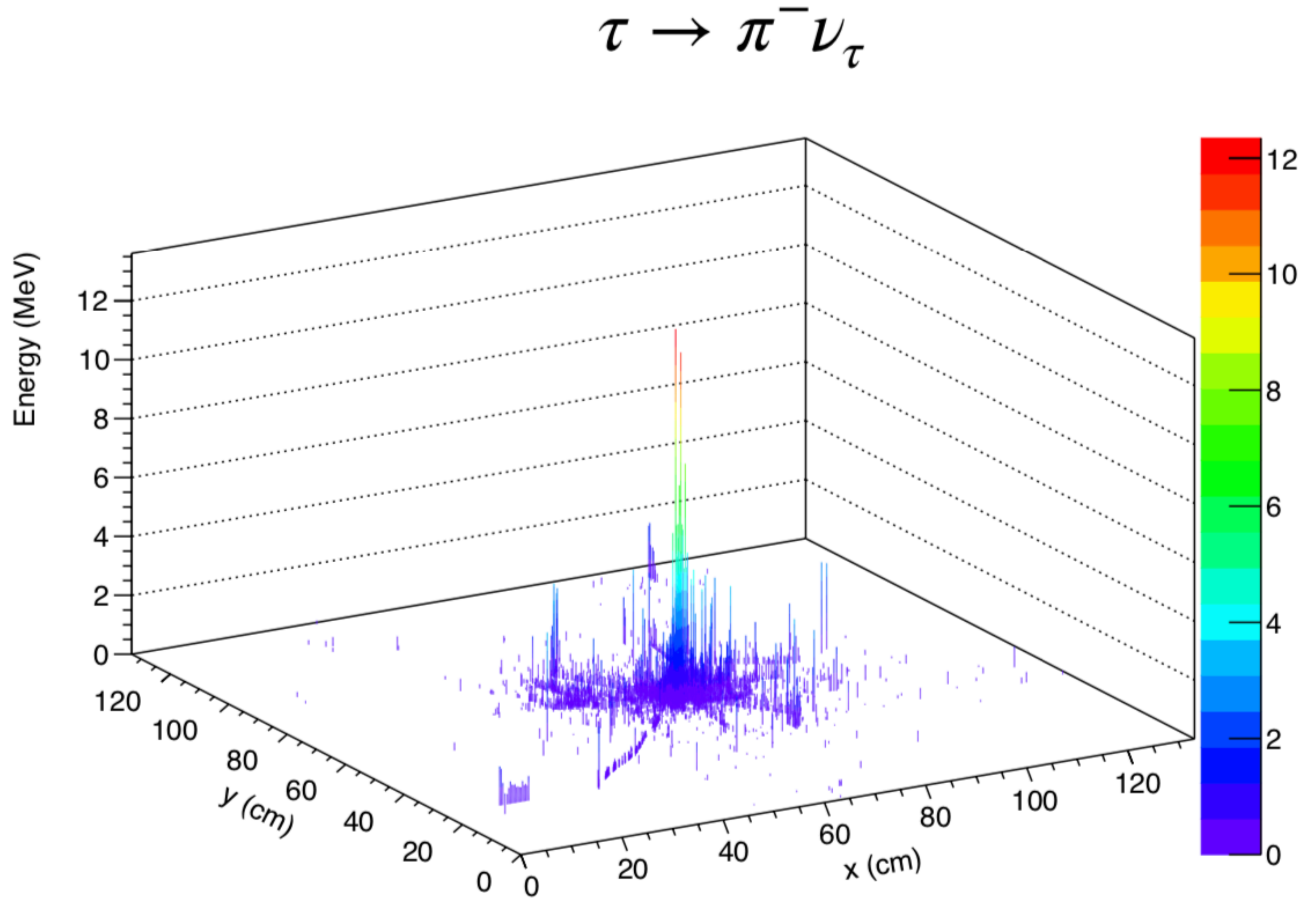
VS

pp → $\gamma_d \gamma_d$ → displaced dark-photons → 2 displaced jet

CONVNET ON FPGA T IDENTIFY TAU DECAYS IN FUTURE GENERATION CALORIMETERS



Fiber pattern *RD52*

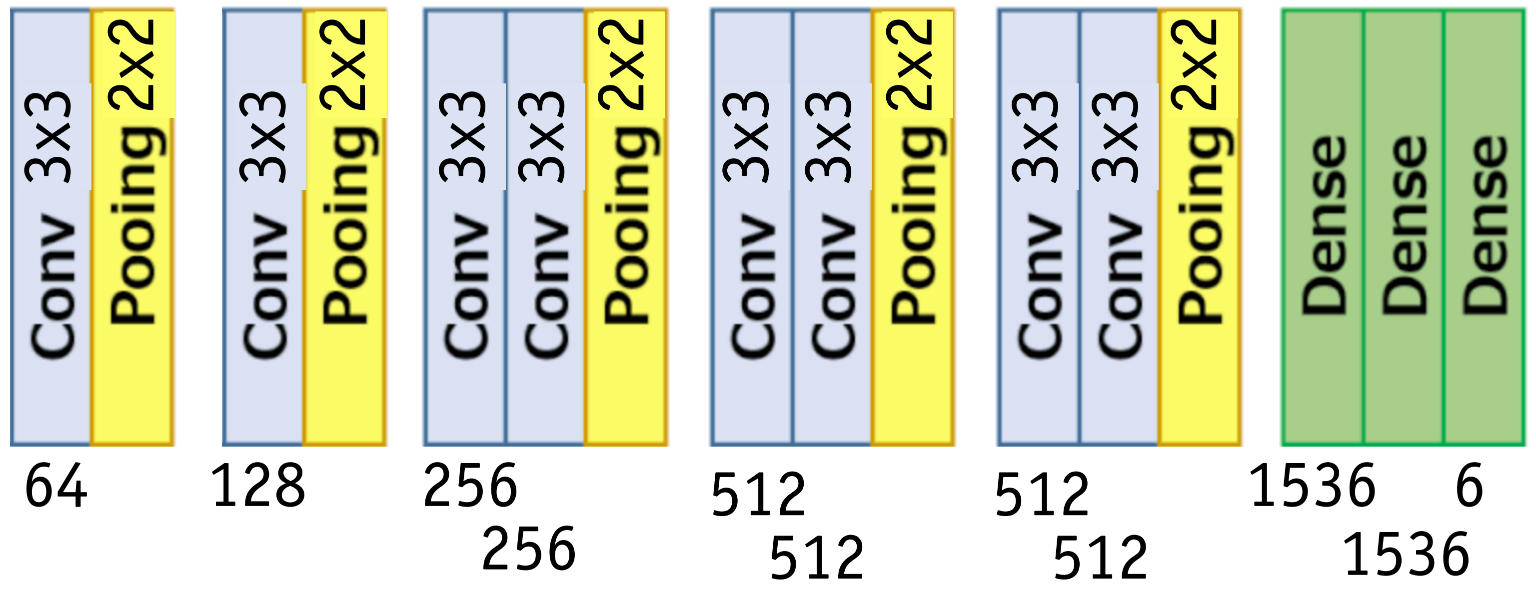


RNN

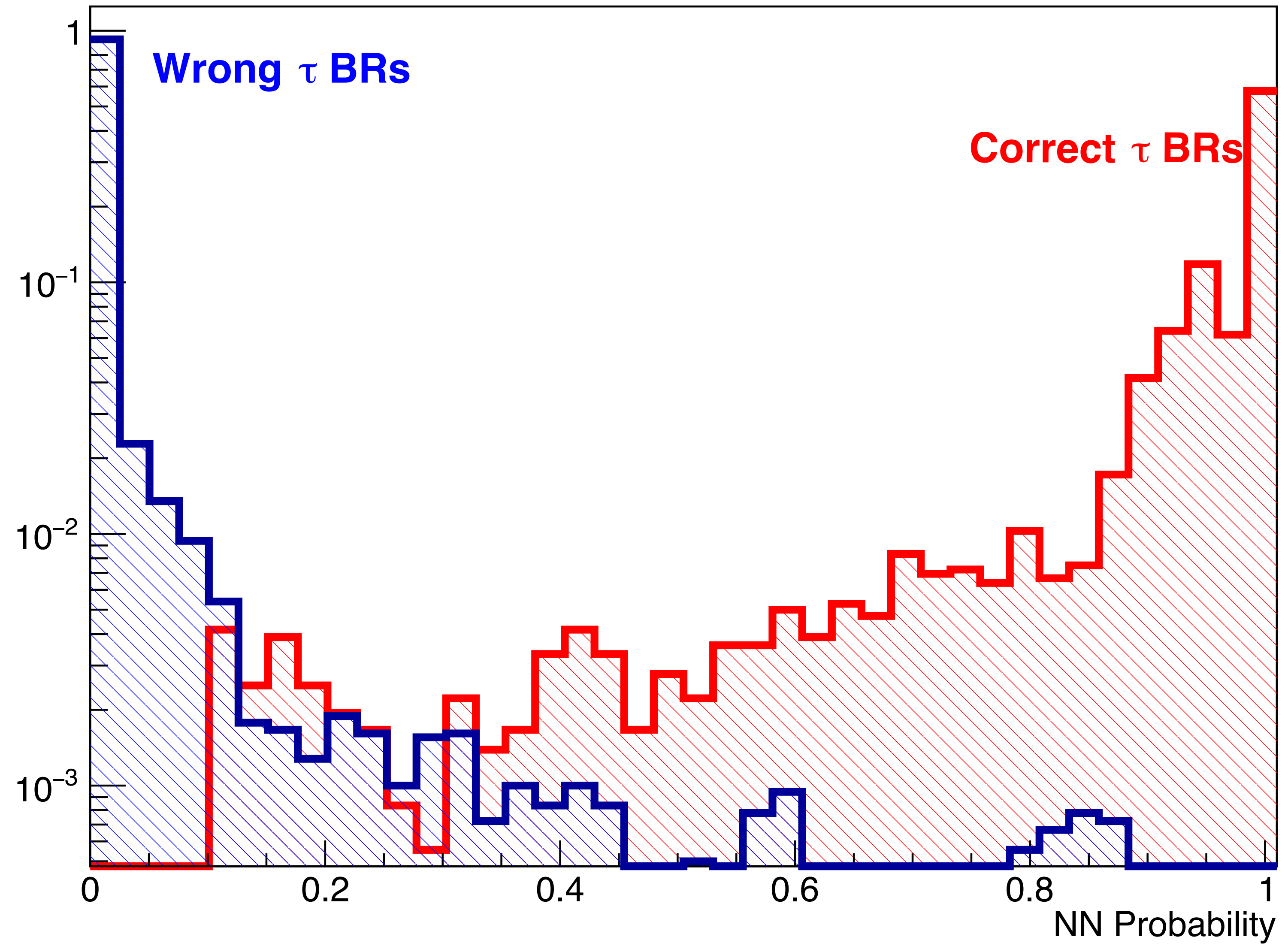
CNN

CNN+RNN

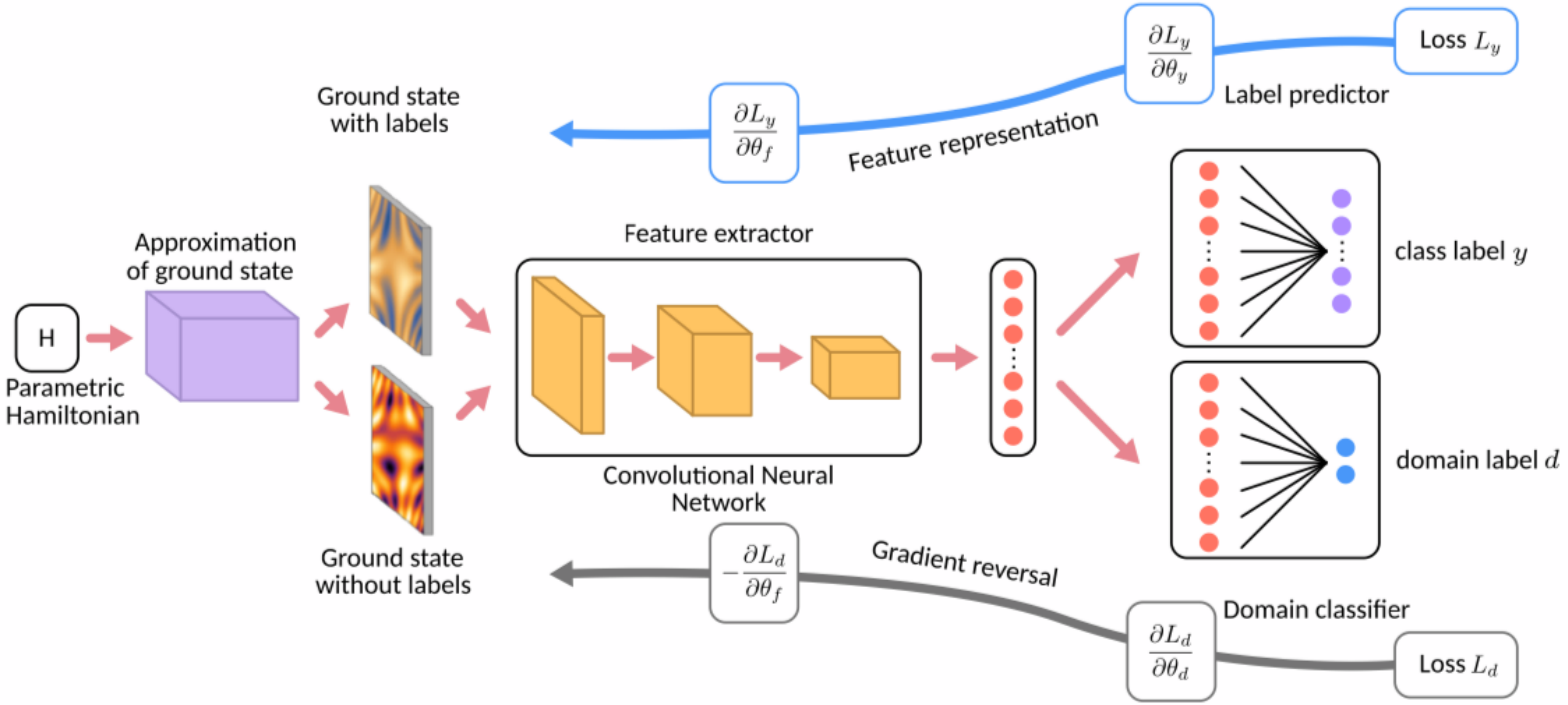
111x111x10
input

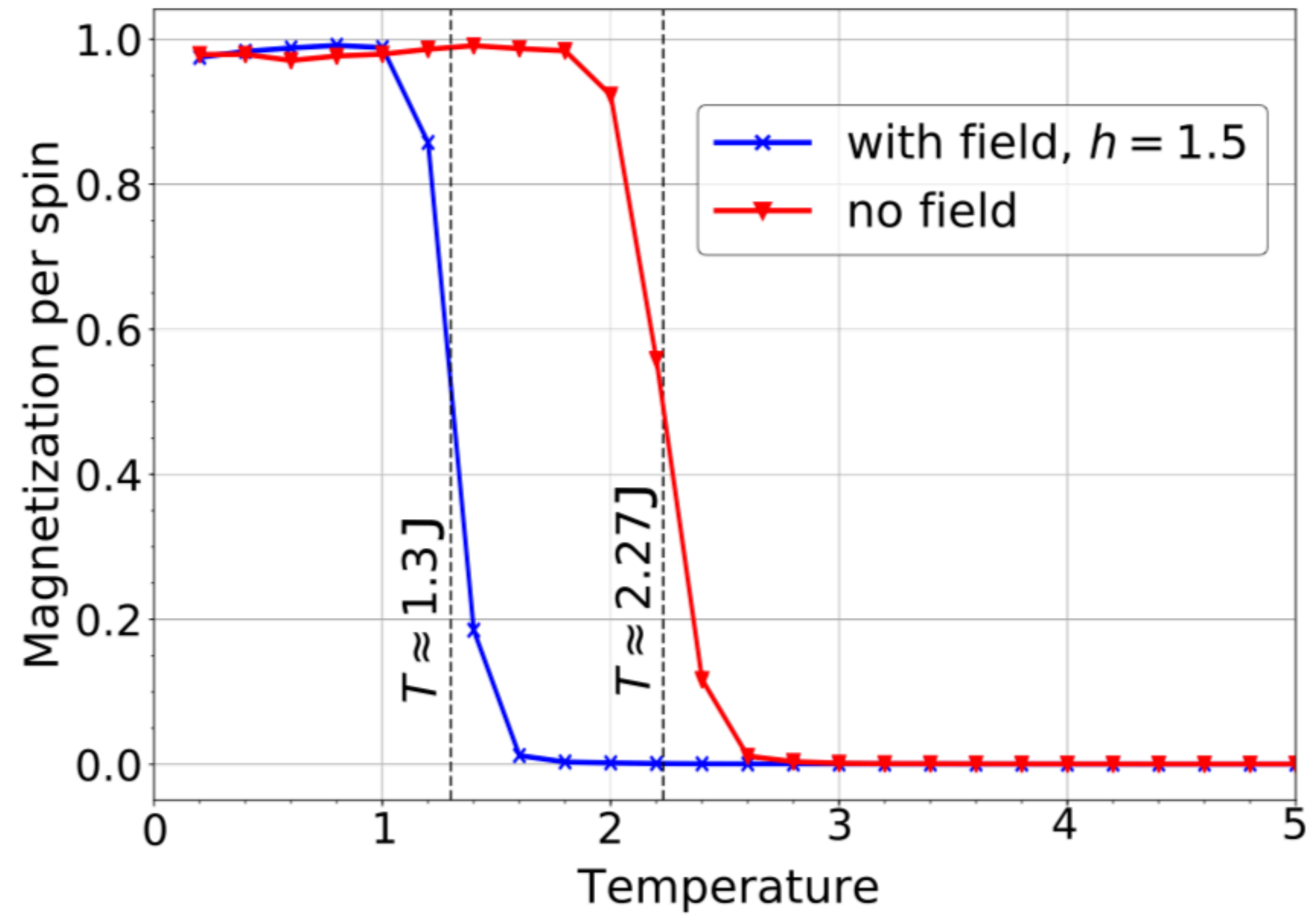


6 classes
probability
output



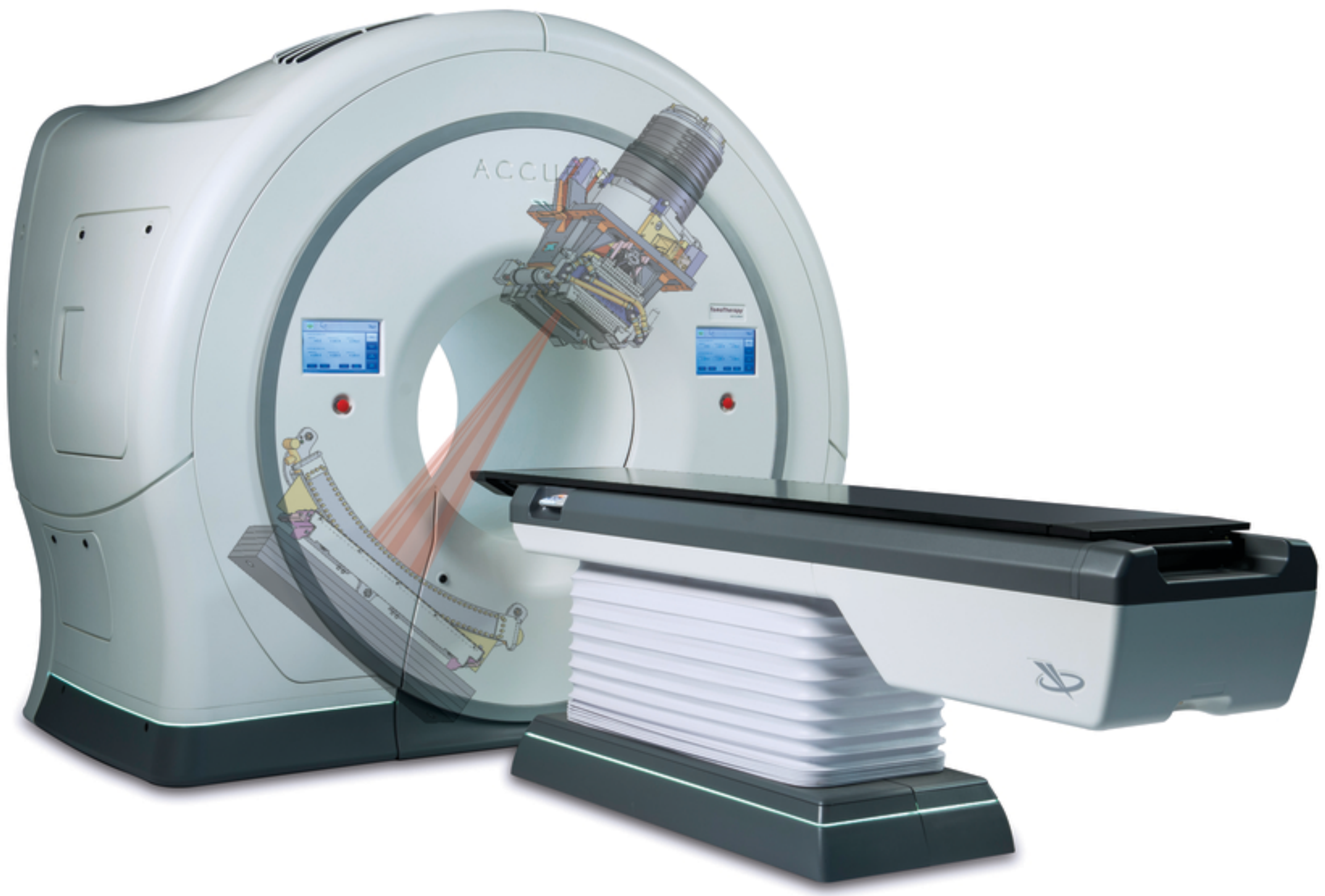
ADVERSARIAL CNN FO RTHE IDENTIFICATION OF PHASE TRANSITIONS IN CONDENSED MATTER ...



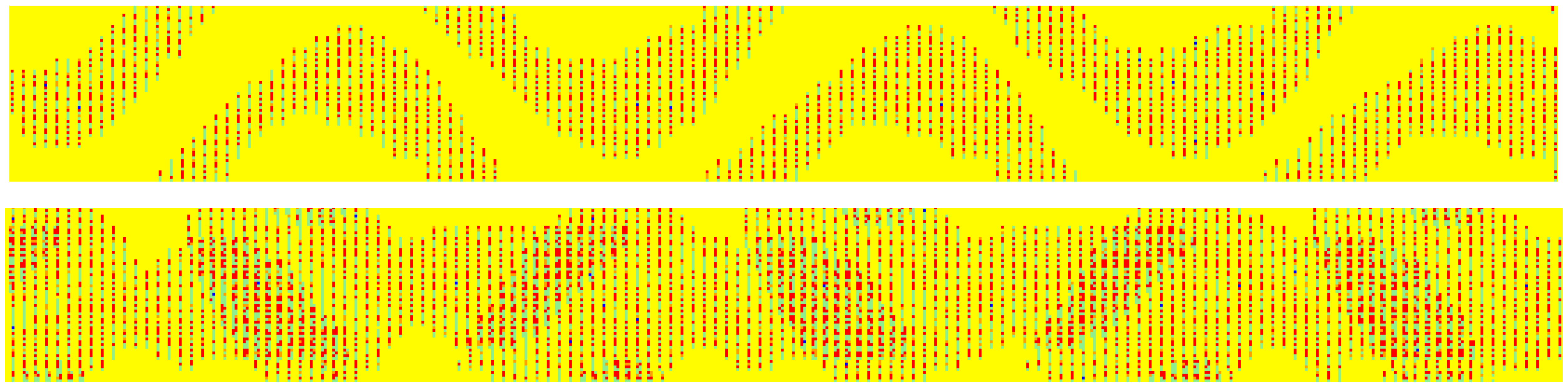


DEEP LEARNING FOR THE MODELLING DI COMPLEX TRANSFER FUNCTIONS

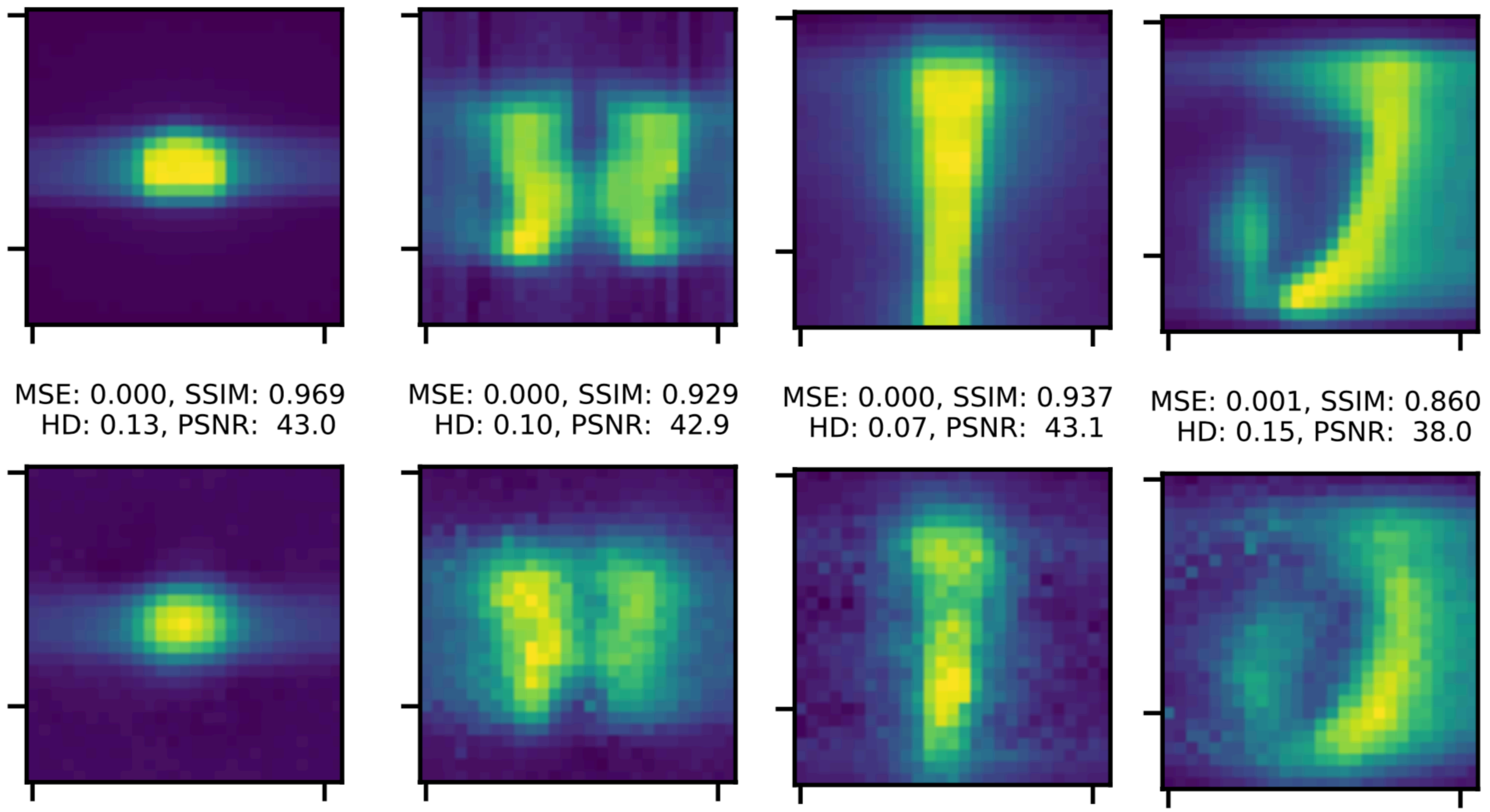
tomotherapy delivered dose as a function of the treatment plan



SINOGRAM



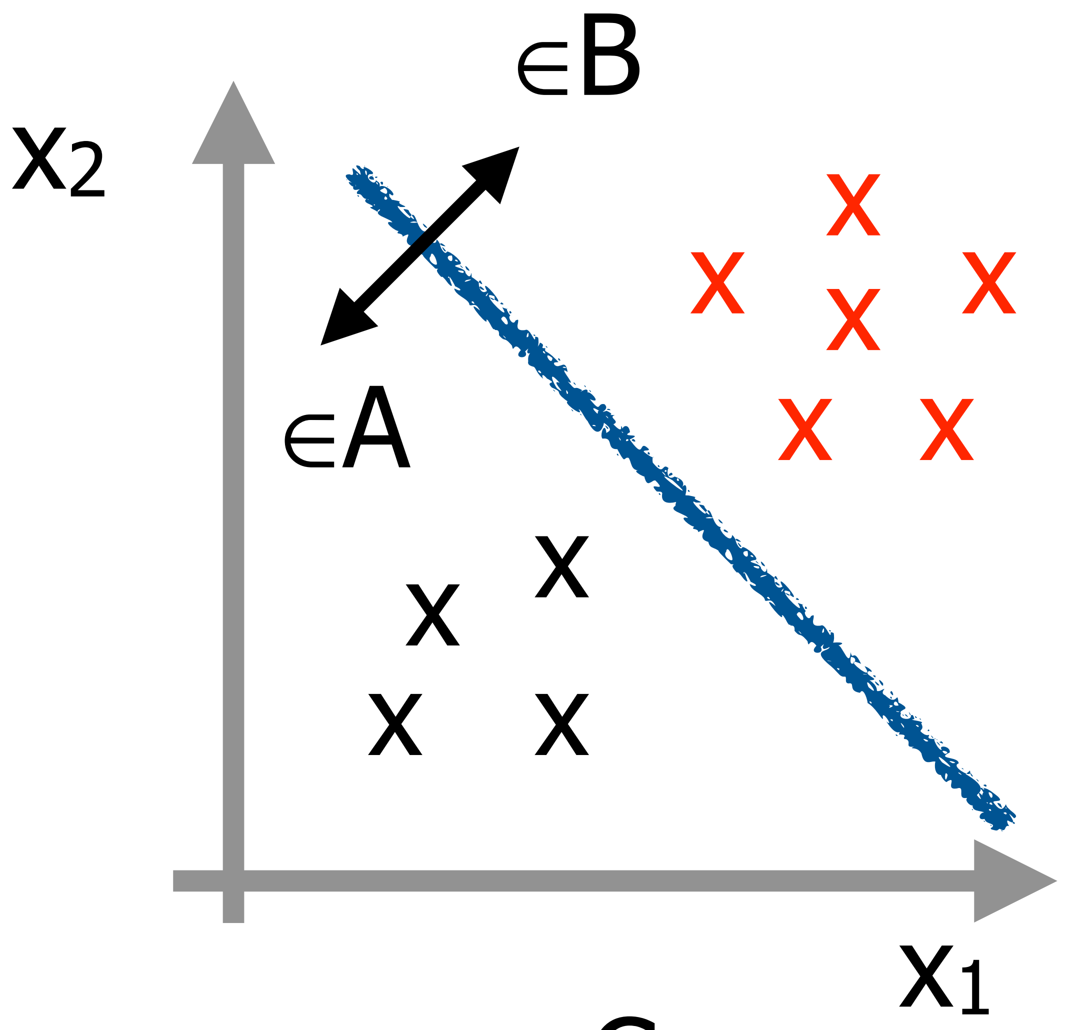
CNN+DNN → DNN



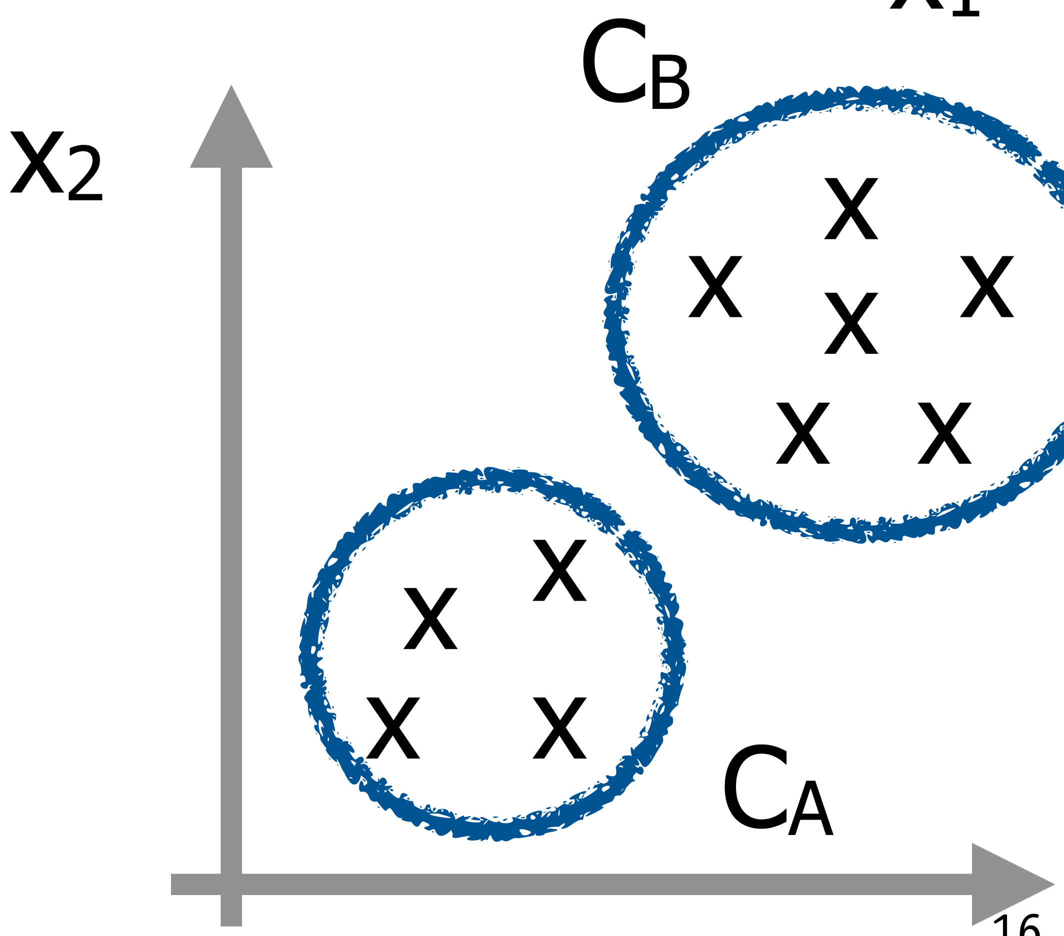
LEARNING PARADIGMS

- Learning algorithms can be divided in different categories that defines which kind of experience is permitted during the training process

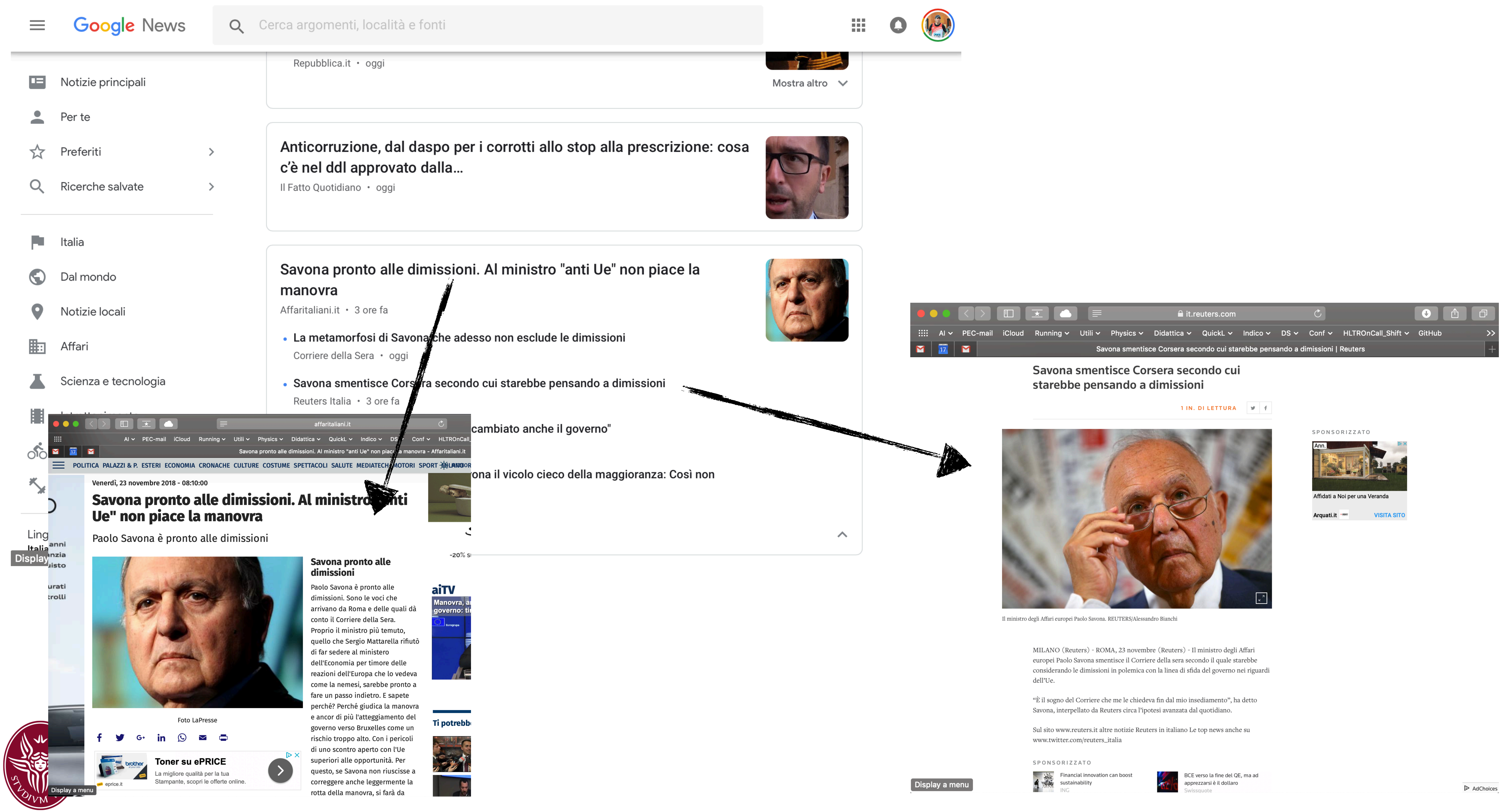
- supervised learning (i.e. there is a teacher):
  - for each example of the training set is provided the true answer (for example the corresponding class) called label
  - Typical target of the training process: to minimise the classification error or the accuracy



- unsupervised (or better: auto-supervised) learning:
  - no explicit information on the true answer for the training set examples is given
  - typical target of the training process: create groups / clusters of the input objects, generally on the base of similarity criteria



UNSUPERVISED LEARNING ALGORITHM EXAMPLE: GOOGLE NEWS

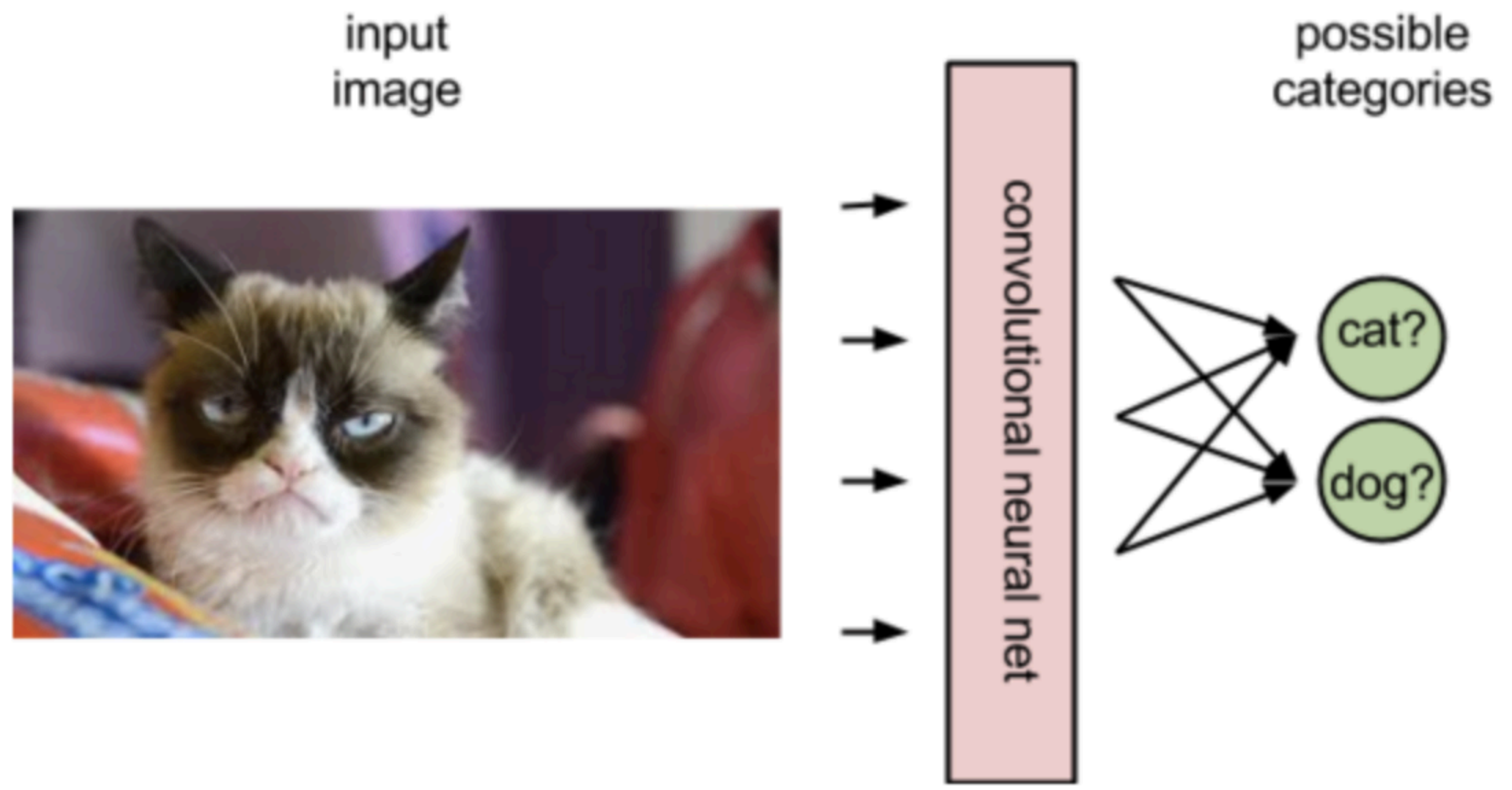


- Reinforcement learning:

  inspired by behavioral psychology: is not used a fixed set of examples/experiences, but the algorithms adapts to teh ambient with which interacts via a continuous feedback between system and examples and through the distribution of a sort of reward (reinforce) that acts on the performance measure P

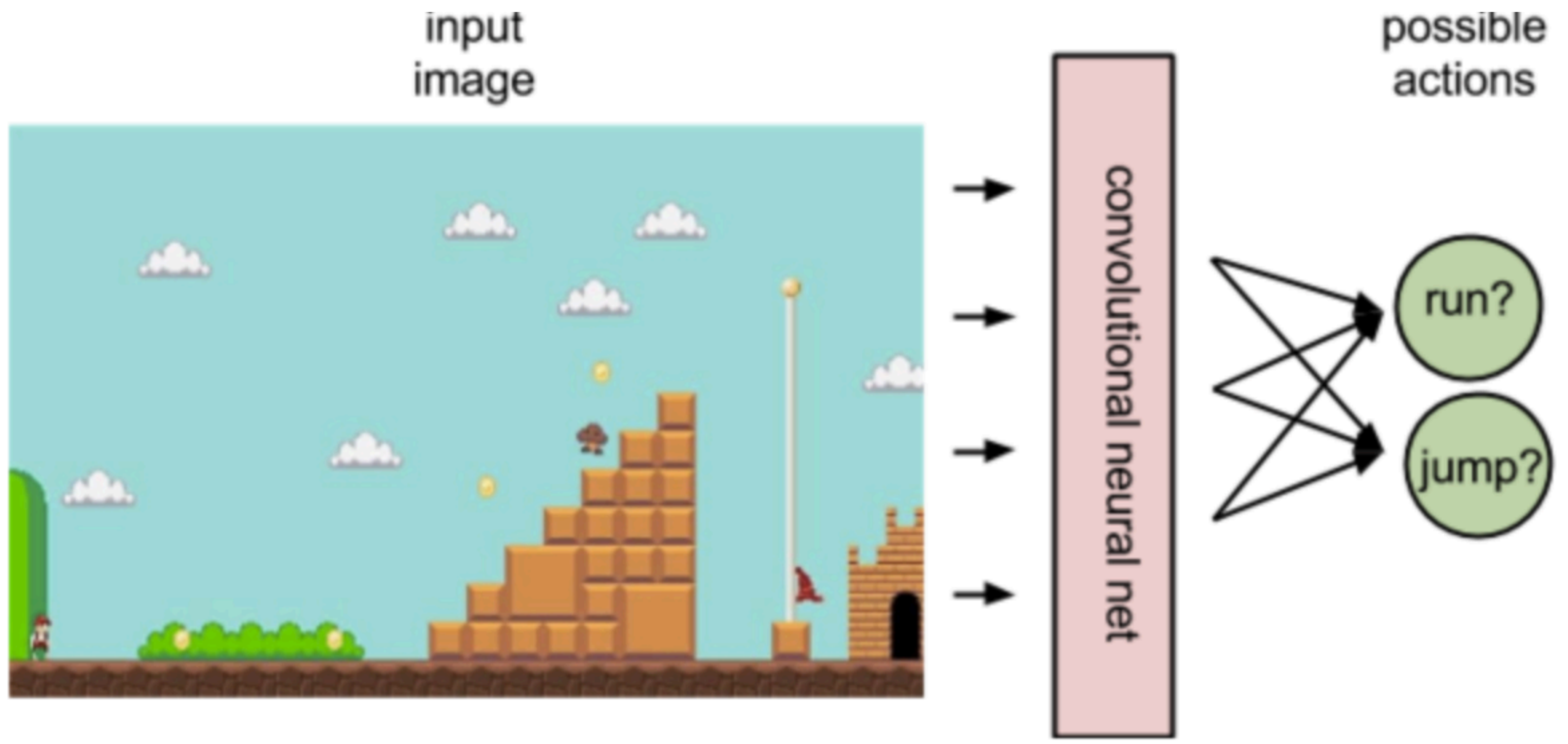
Solve the complex problem of relating instantaneous actions with the effect that they may produce at a later time

example: to maximise the score in a game that develop over multiple moves



Supervised ConvNet

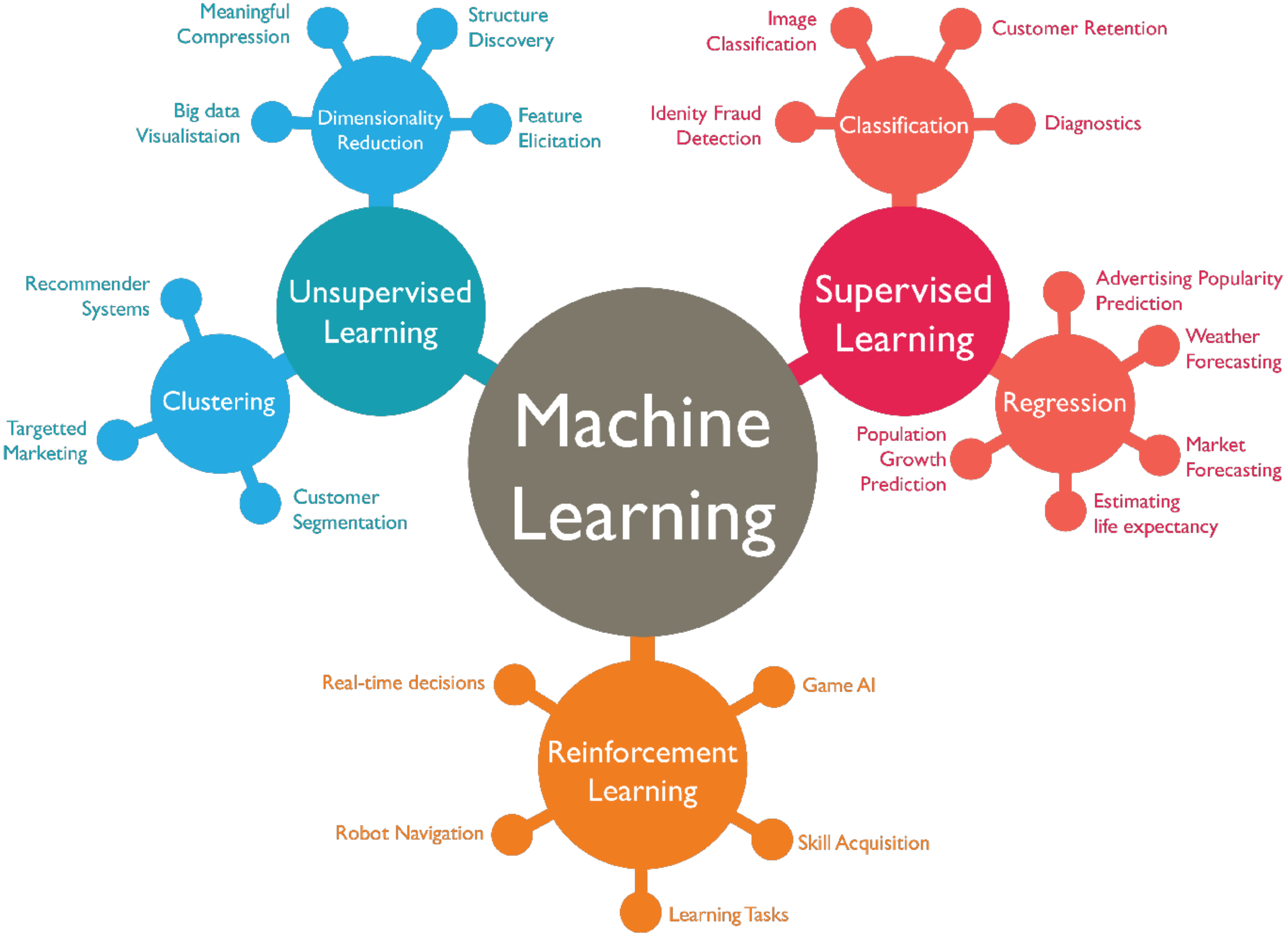
Associate a label to an image



Convolutional agent

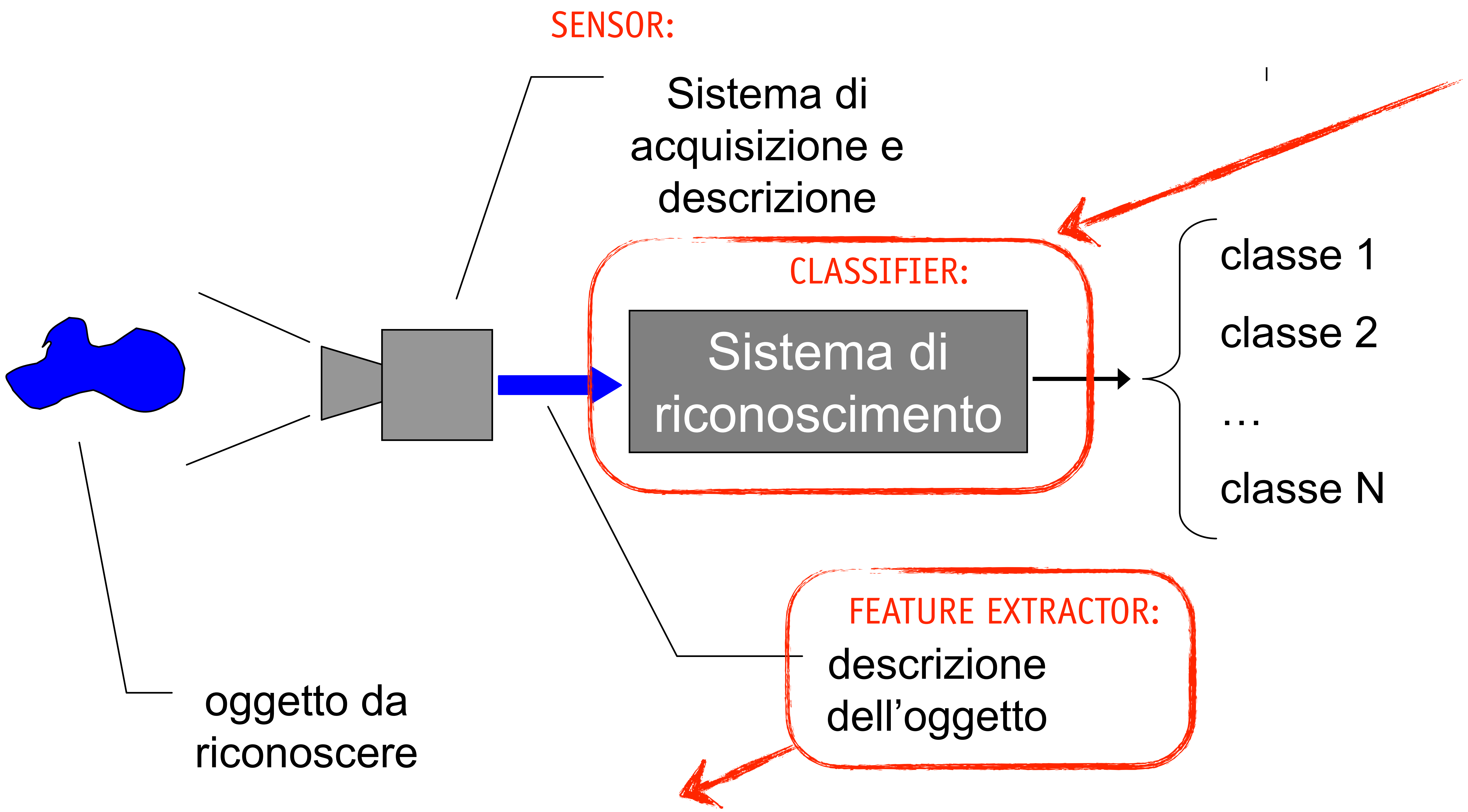
Maps a state to the best possibile action

ML: LEARNIGN PARADIGMS AND TASKS



CONCEPTUAL SCHEME OF THE SIMPLEST CLASSIFICATION SYSTEM

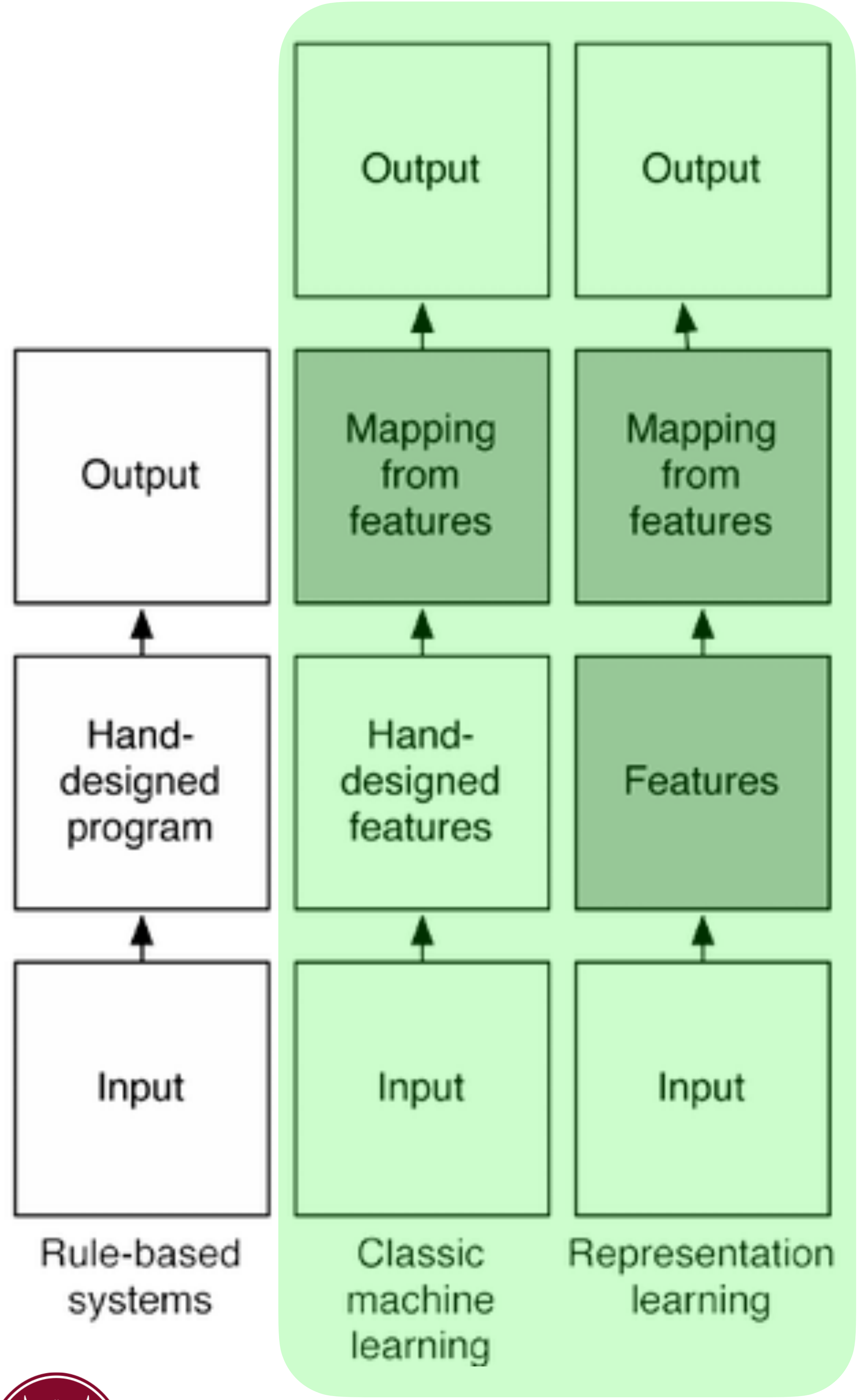
- Given the description of an object that can belong to N possible classes, task for the system is to assign the object to one of the classes (o to assign a probability to each class) by using the knowledge base build during the training phase



the features are used as input to a recognition algorithm that on the base of such features classifies the object

The feature estractor present to the recongition system a rapresentation, i.e. a set of measures (features) that characterise the object to be recognised and facilitate the task

LERN THE DATA REPRESENTATION

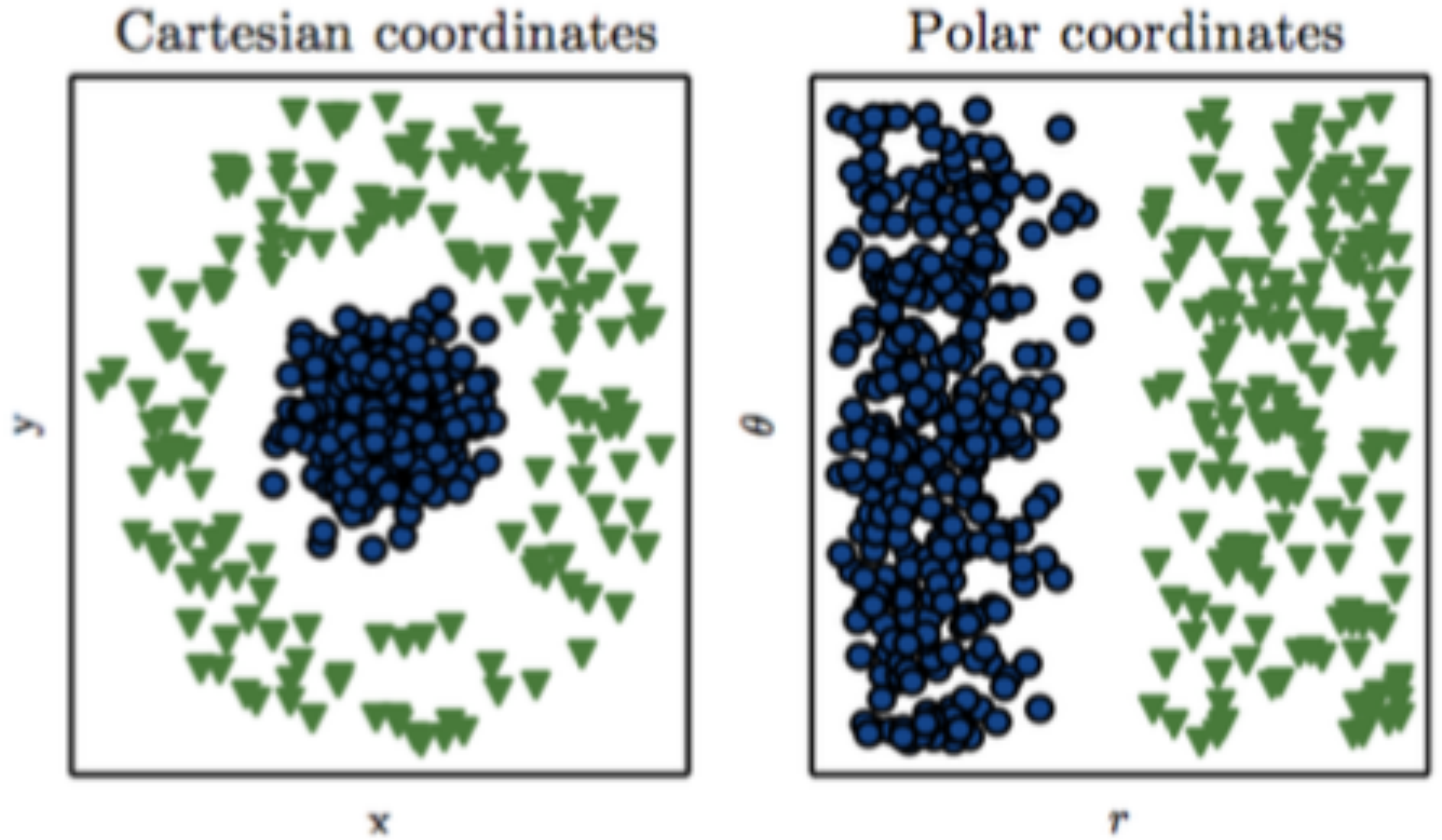


in first generation (classic ML): the feature set were build and chosen by the operator on the base of prior knowledge of the problem itself

- human: identify best features
- algorirthm: identify the best mapping between features and output

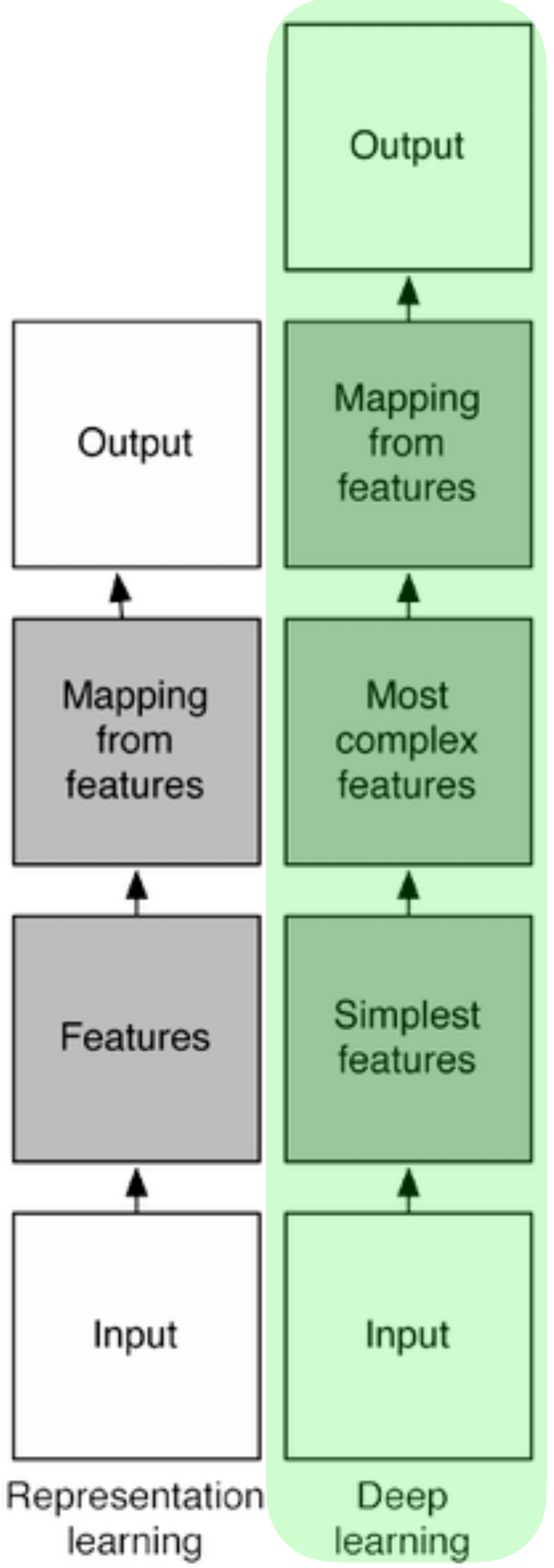
second generation ML: Representation Learning

- the algorithm scope is expanded by performing also the task to find in an automatic way a better representation of the data with respect to the one available with the input features



DEEP LEARNING (DL)

- the traditional ML algorithms were not very “creative” in finding better representations
- basically they just searched the best possible transformation in a predefined set of operations called ”hypothesis space” of the algorithm. Search guided by the training examples
- The Deep Learning evolution solve this limitation by organising ideas and concepts in a hierarchical way and building new complex representations based on simpler ones
  - example: a person face can be presente by combining simpler features: eyes, mouth, hears …, that can be represented in trun by combining basic features: edges, contours, lines, …
- DL == HIERARCHICAL REPRESENTATION LEARNING

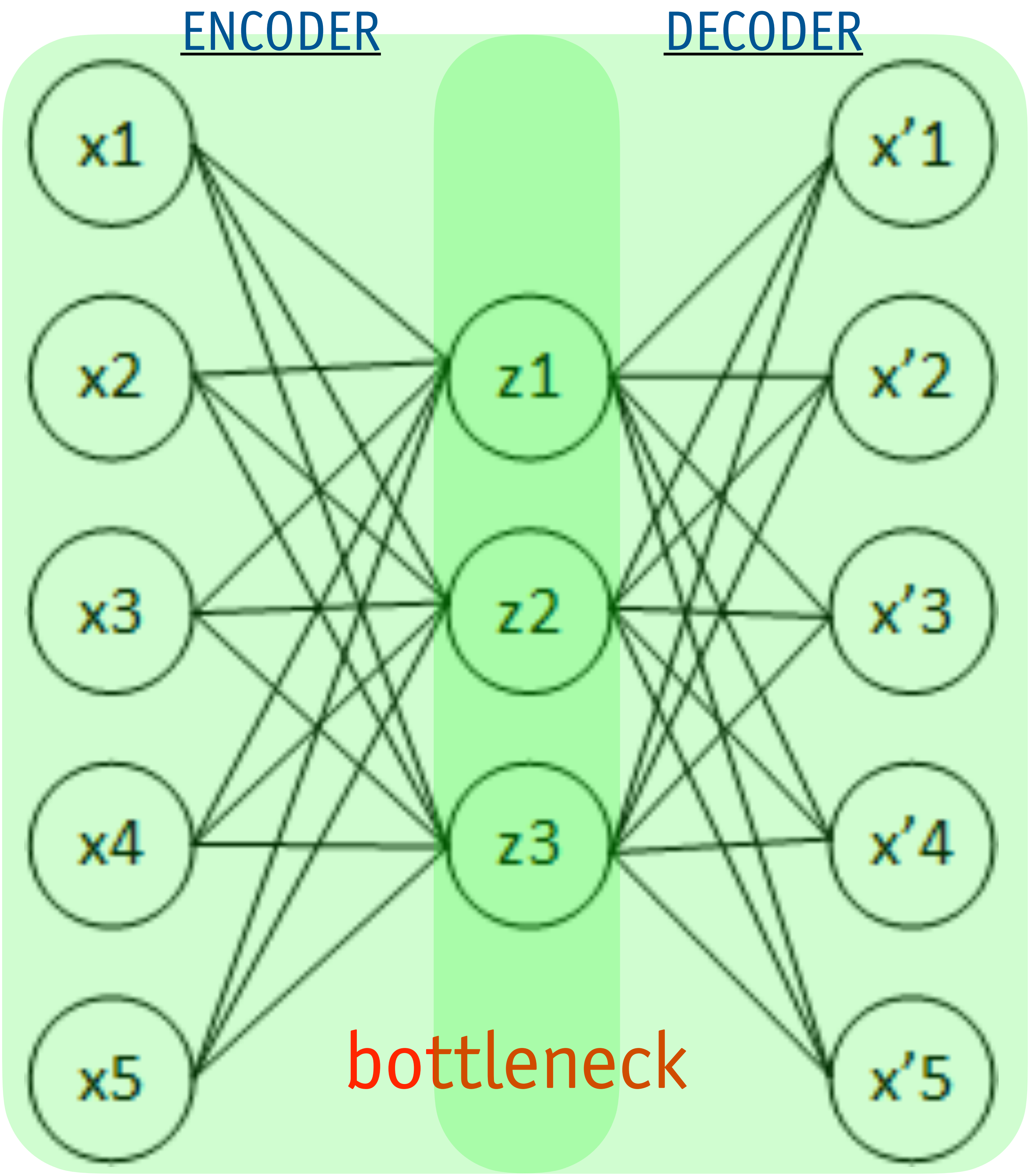


Extremely powerful, but requires huge training sets
and a lot of computing power …

AUTOENCODER: A BASIC EXAMPLE OF REPRESENTATION LEARNING

- non-supervised algorithm that try to identify common and fondamentali characteristic in the input data
- combines and encoder that converts input data in a different representation, with a decoder that converts the new representation back to the original input
- trained to output something as close as possible to the input (learn the identity function)

input v(5)

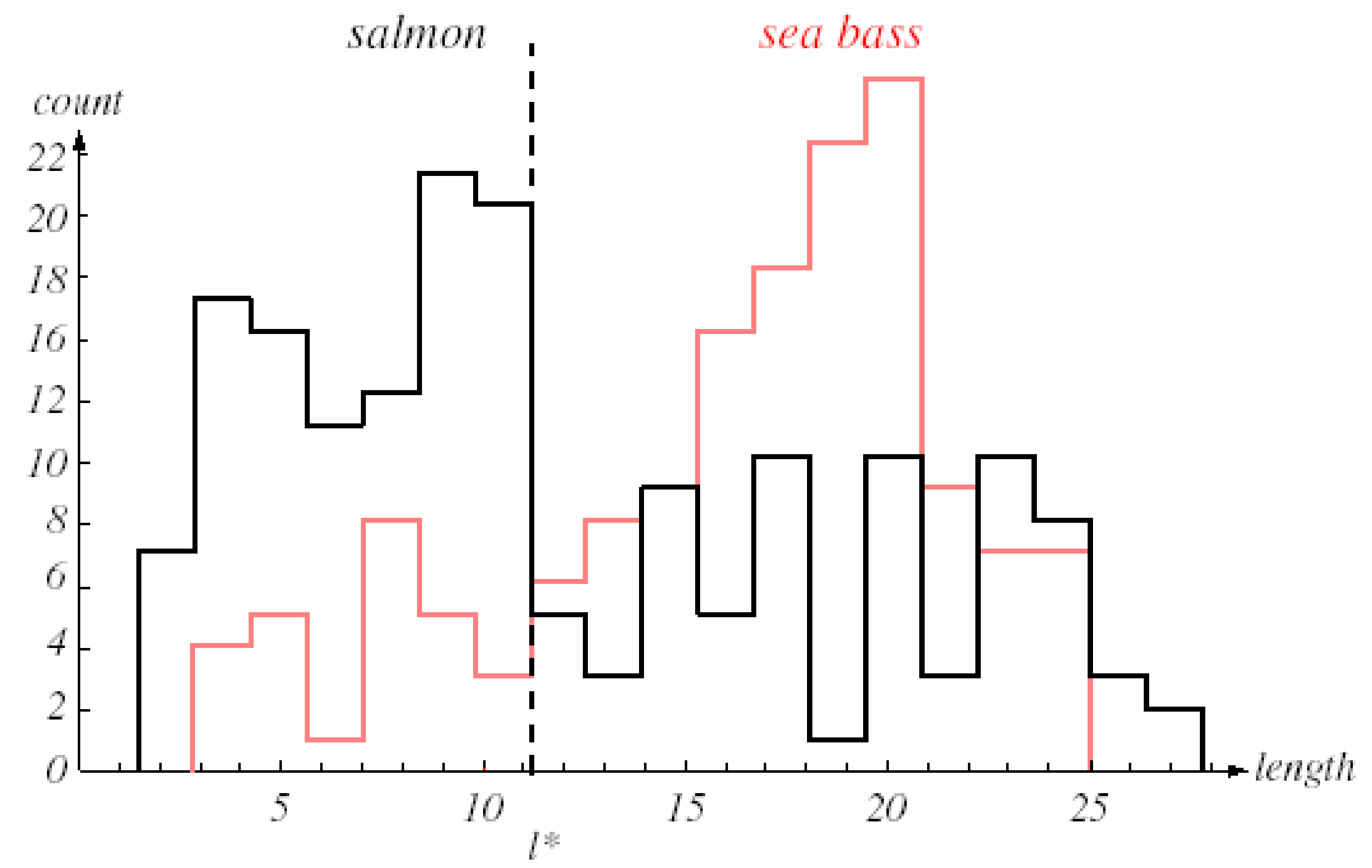


output = input

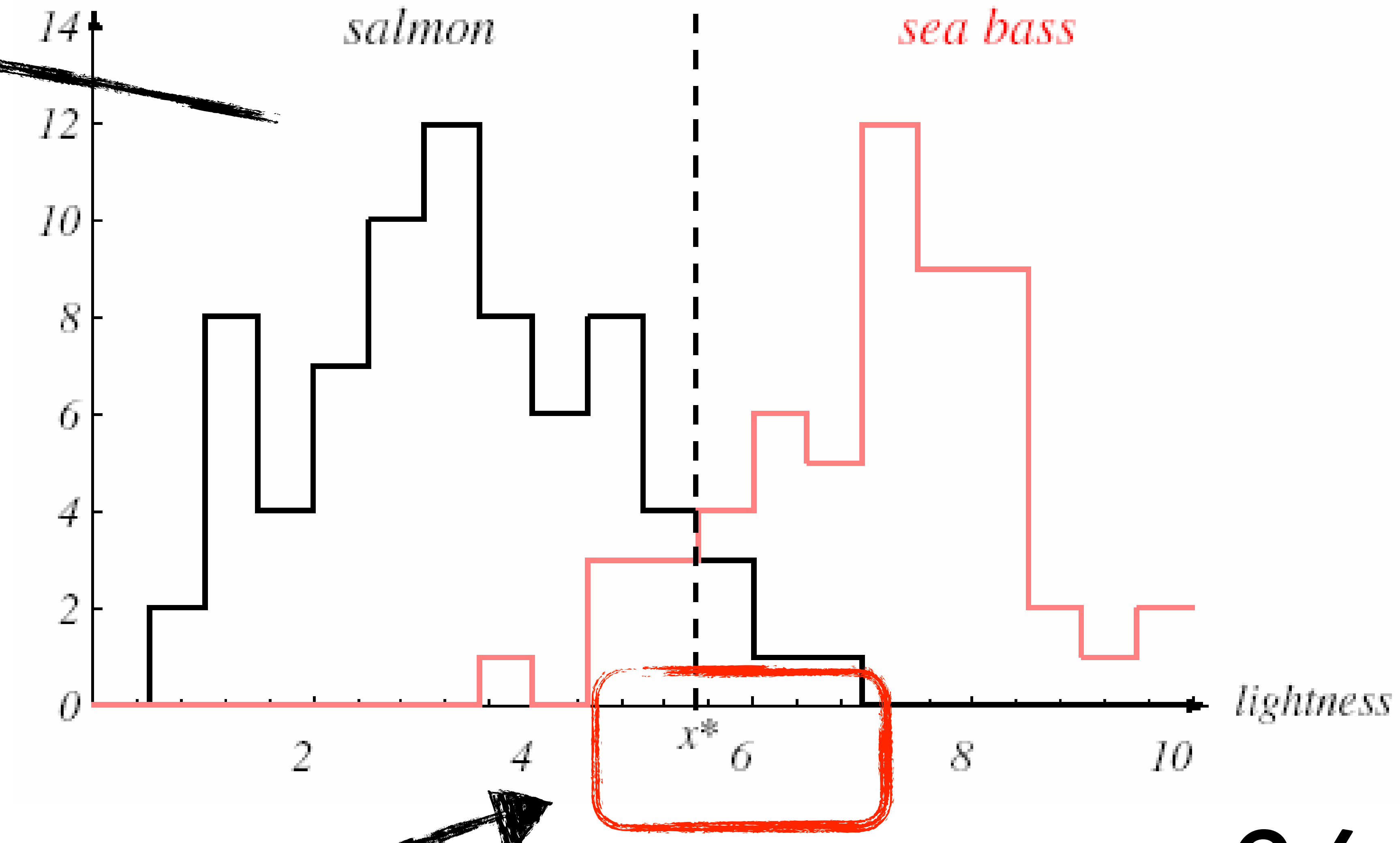
- "trivial" unless to constrain the network to have the hidden representation with a smallare dimension of the input/output
- in such case the network build (learn) "compressed" representations of the input features: $x \in R^5 \rightarrow z \in R^3 \rightarrow \cdots$

DECISION BOUNDARIES

- let's assume that we have found that the two best features for our classification task are: length e lightness
- which one we should use for the classification? Which threshold?
- to decide this we make use of the traing set examples



Classification rule:	if x > x*:	object ∈ class A
	else:	objetc ∈ class B

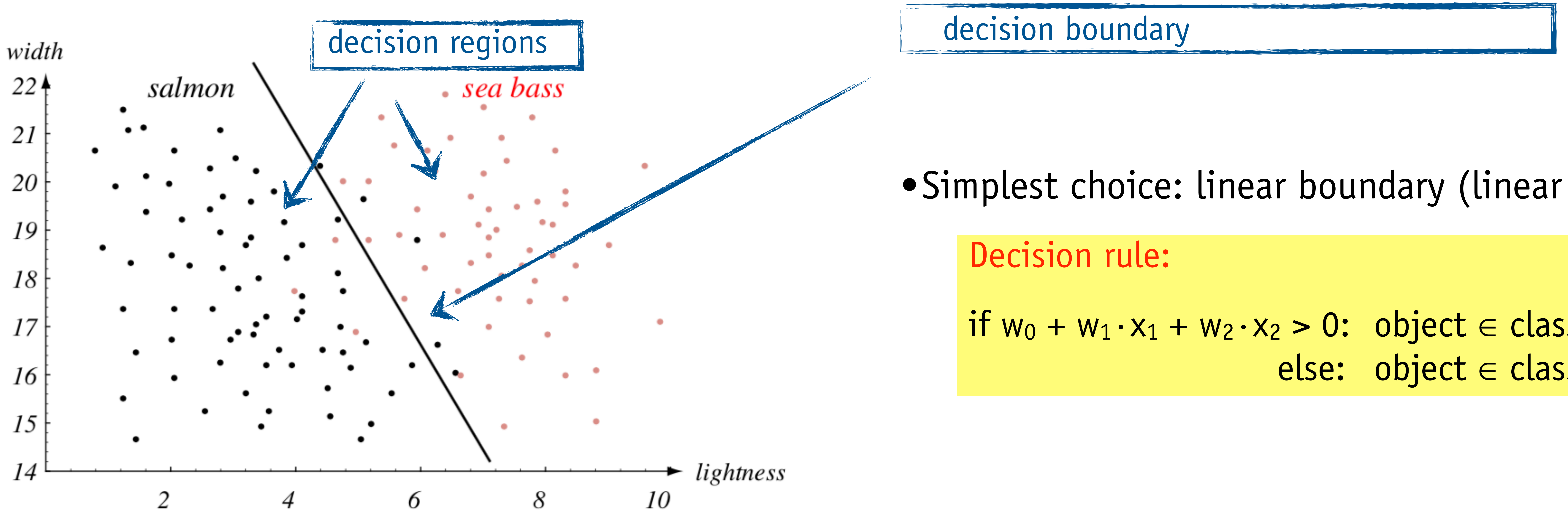


the threshold x* is chosen in order to optimize an appropriate performance measure

example: accuracy, probability of misclassification, statistical risk ...

DECISION BOUNDARIES

- to improve P a better strategy woudl be to use more than one feature at the same time
- The classification problem becomes the problem to find the best partition of the feature space, so that the classification error is the smallest one



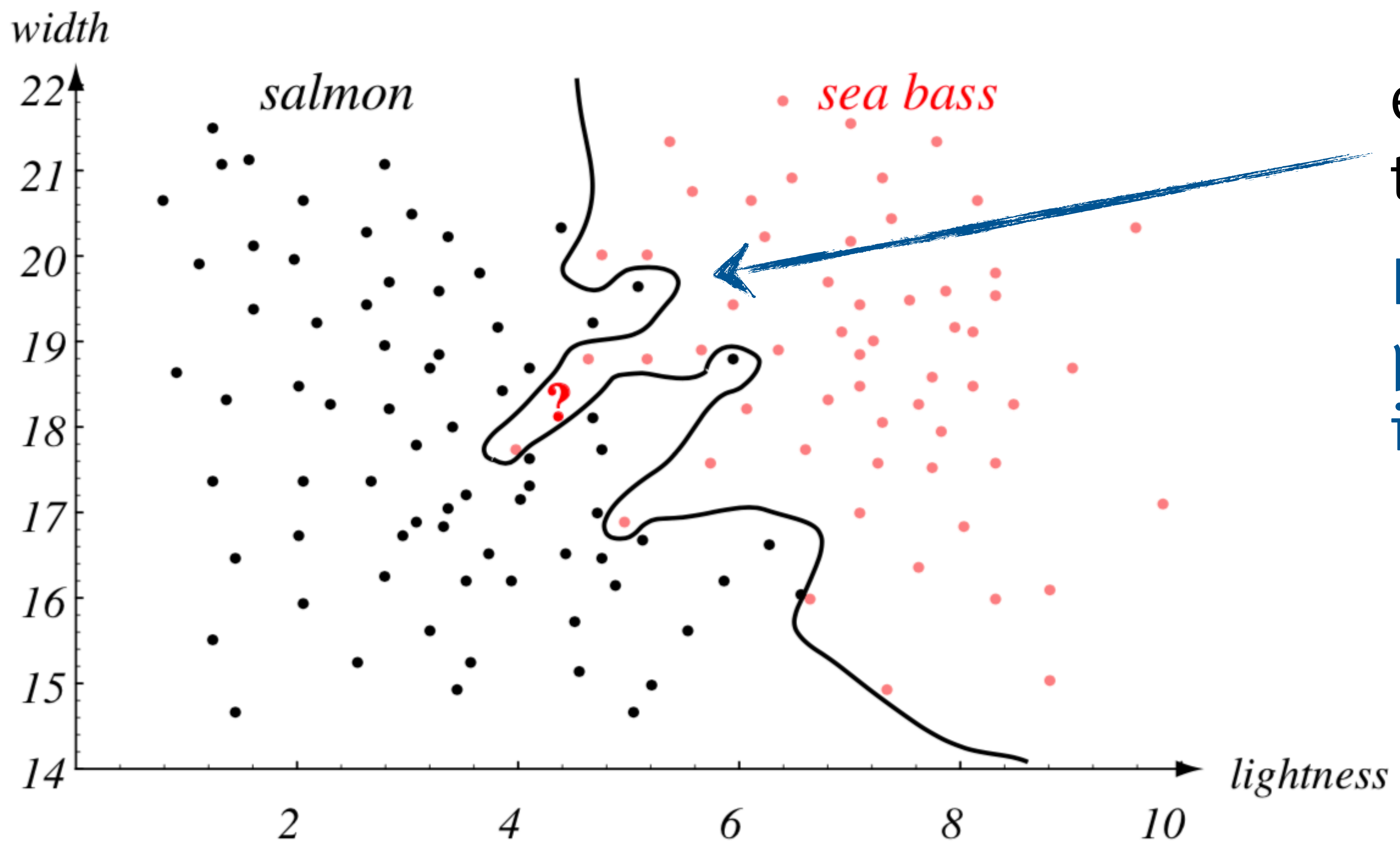
- Simplest choice: linear boundary (linear classifier)

Decision rule:

if $w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 > 0$: object $\in$ class A
else: object $\in$ class B

COMPLEX DECISION BOUNDARIES ...

- question: it is possible to get rid of all errors with a complex decision boundary?



example: this boundary correctly classifies all the events of the trining set

PROBLEM: this way we are NOT guarantee a good performance of the algorithm when applied to events from independent samples wrt the training set (overfitting)

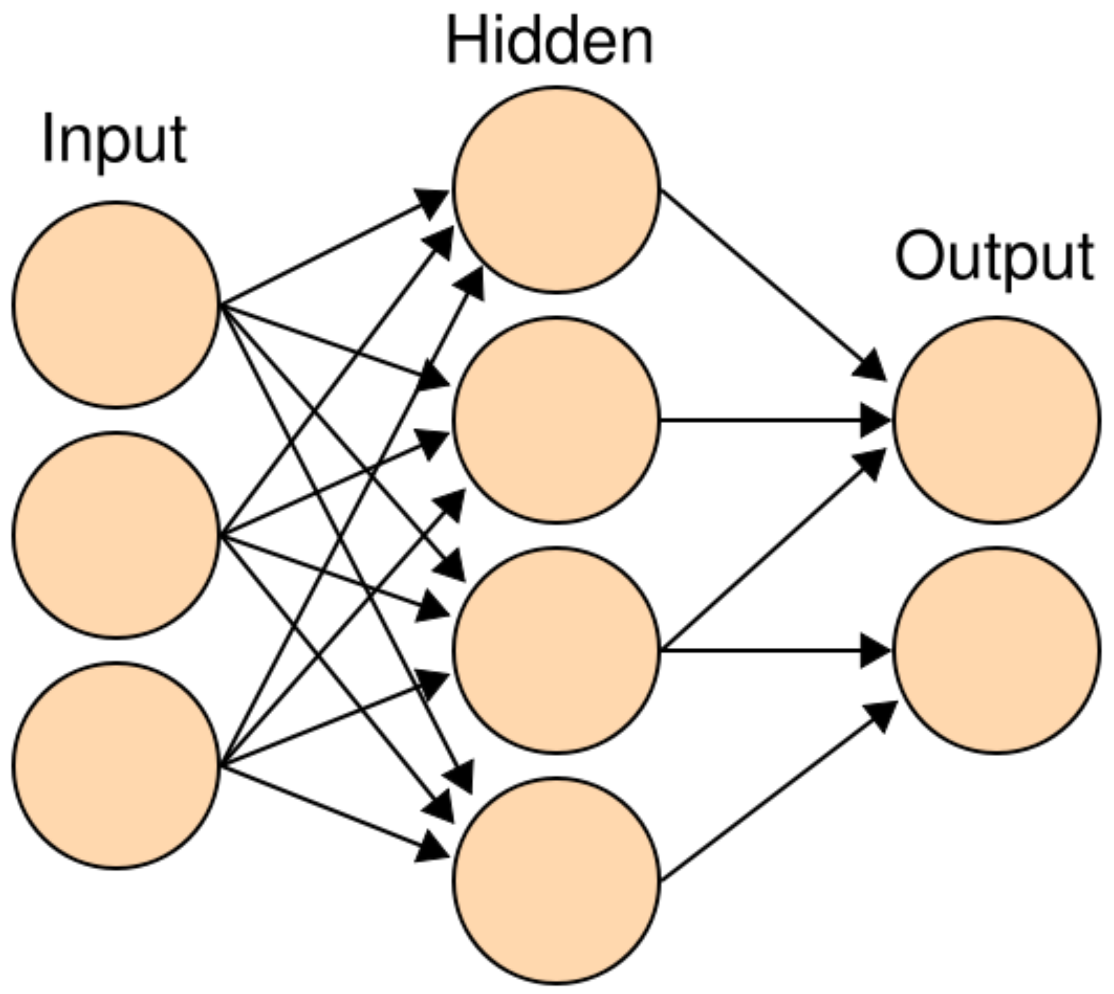
the decision boundary is sensitive to the statistical fluctuation in the training set

- it is always preferable to accept a certain margin of error on the trining set if this allows to a better generalisation of the algorithm
- this aspect is called generalisation problem, and one of the crucial aspect in the design and training of any ML algorithm

ARTIFICIAL NEURAL NETWORKS

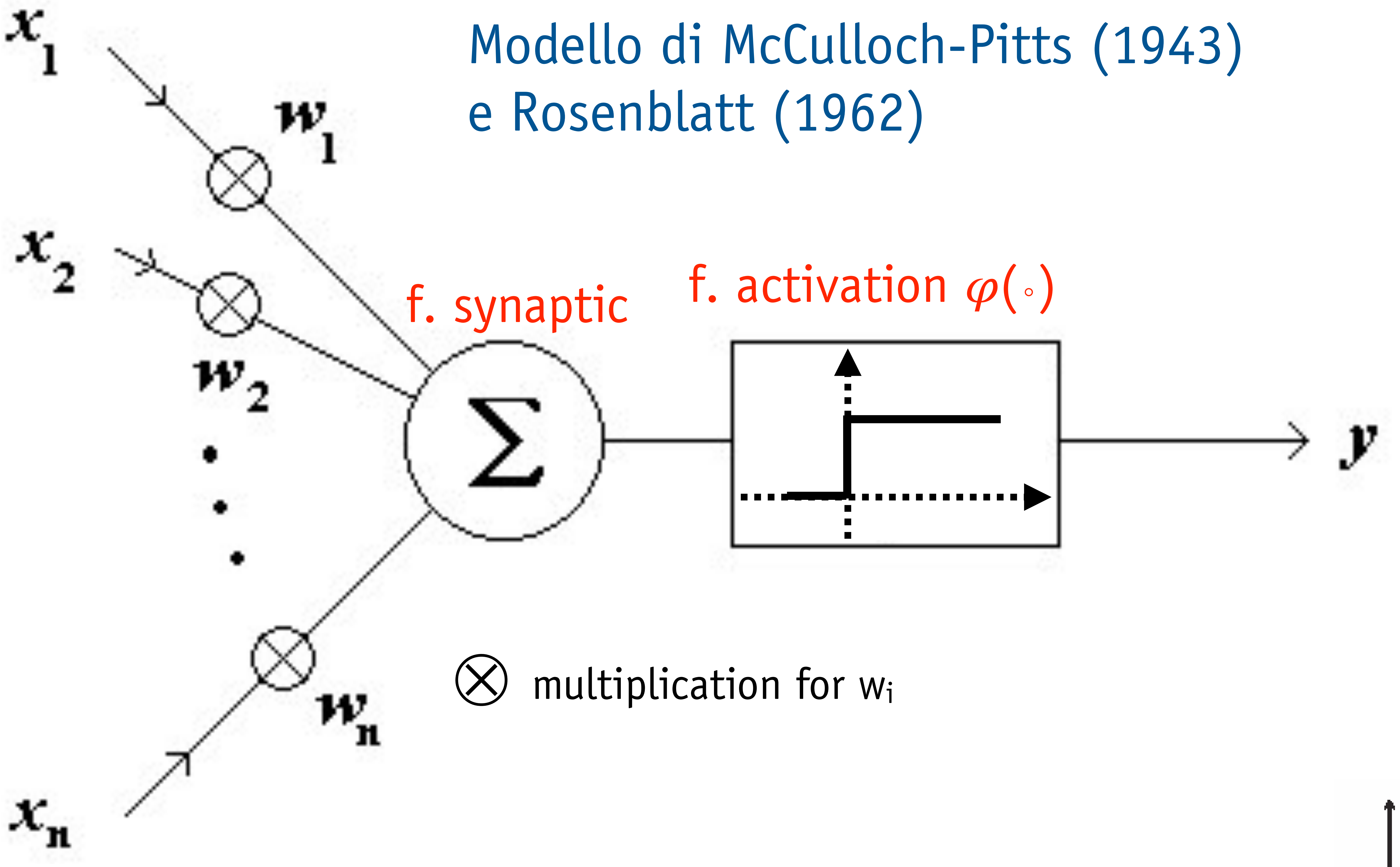
- the most popular approach to machine and deep learning to date
- an ANN is a mathematical model able to approximate with high precision any functional form

  - based on an interconnected group of identical computational units (neurons)
  - process input information accordino to a connectionist approach: → collective actions performed in parallel by simple processing units
  - behave as an adaptive system: structure dynamically modified during the learning phase based on a set of examples that flow through the network during the training step



  - non linear response obtained by non linear activation functions used as output of each neuron
  - hierarchic representation learning obtained by implementing complex architectures with multiple layers of connected neurons (deep-NN)

ARTIFICIAL NEURON MODEL



Modello di McCulloch-Pitts (1943)
e Rosenblatt (1962)

f. synaptic

f. activation $\varphi(\circ)$

$\otimes$ multiplication for w_i

Characteristics:

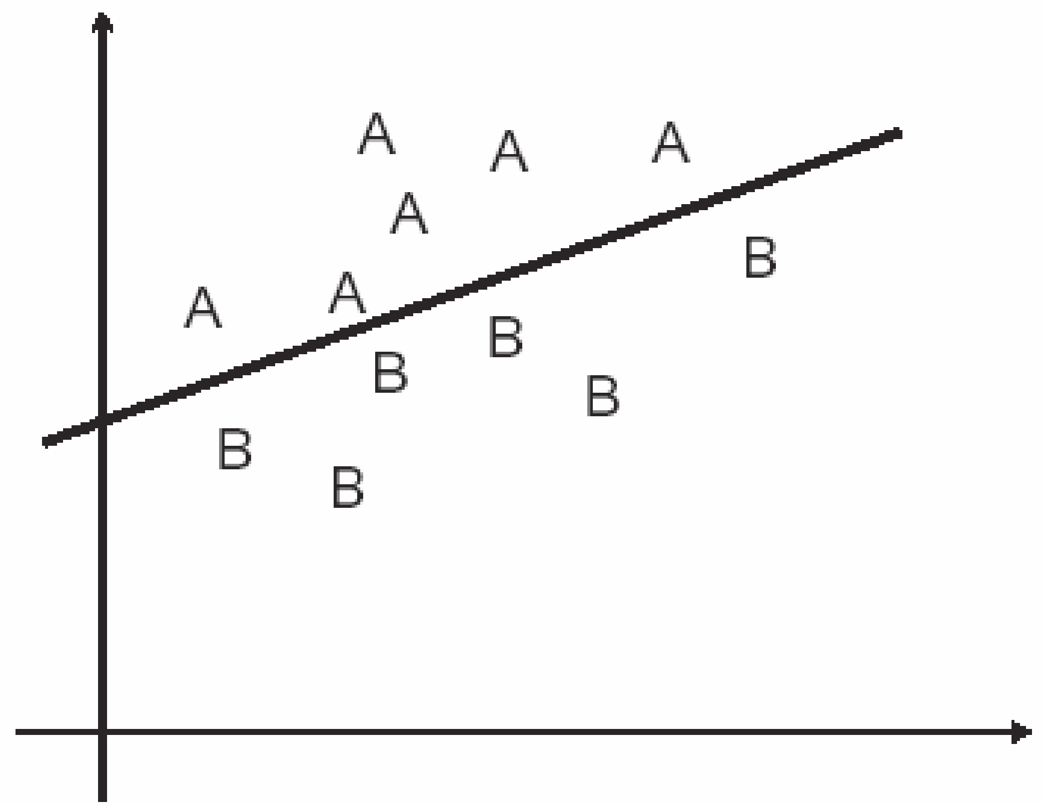
- receives in input n signals x_i and produce an output y given by the composition of a synaptic function:

$$a = \sum_{i=1}^{n} w_i x_i = \mathbf{w}^t \mathbf{x}$$

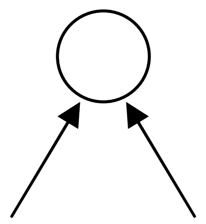
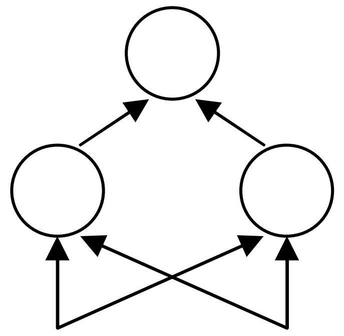
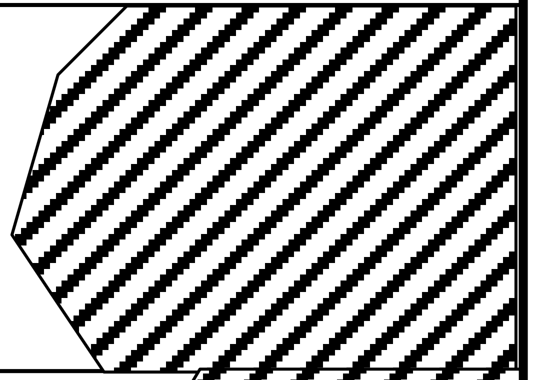
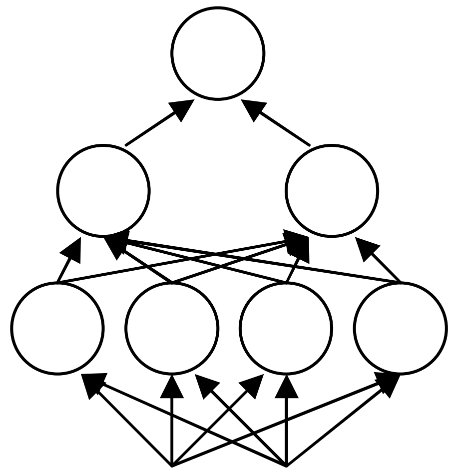
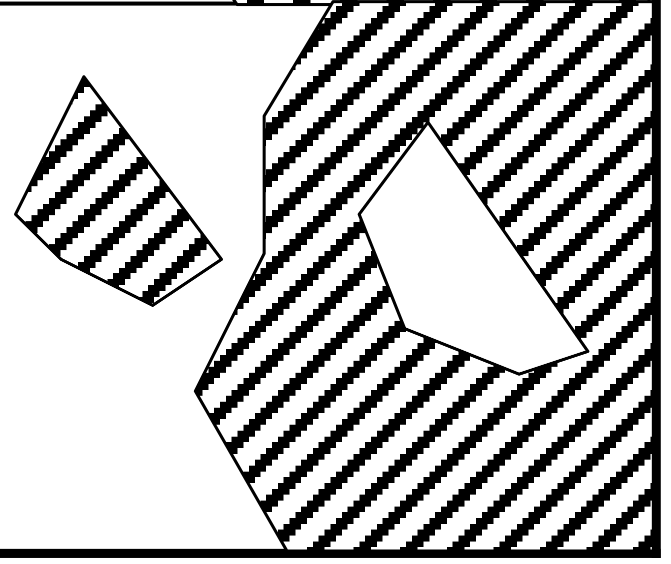
- and an activation function (Heaviside):

$$y = \varphi(a) = H(a - w_0) = \begin{cases} 1 \text{ if } a \geq w_0 \\ 0 \text{ if } a < w_0 \end{cases}$$

with a TLU it is possible to solve problems with linearly separable classes:



COMPLEX SEPARATION REGIONS

Struttura	Regioni di decisione	Forma generale
	Semispazi delimitati da iperpiani	
	Regioni convesse	
	Regioni di forma arbitraria	

Universal Approximation Theorem

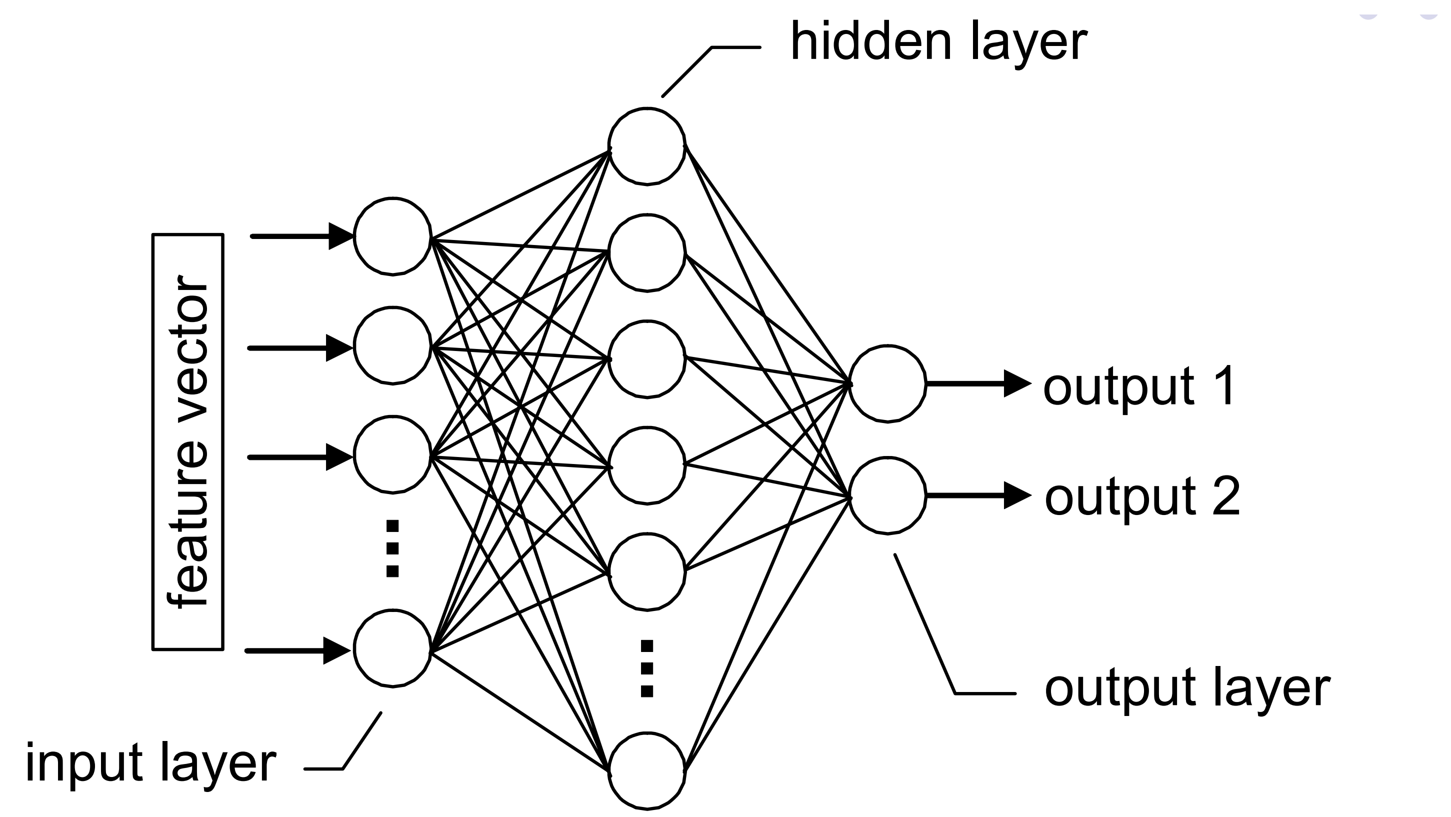
a feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of Rn, under mild assumptions on the activation function

$$F(x) = \sum_{i=1}^{N} v_i \varphi\left(w_i^T x + b_i\right)$$

NOTE: the theorem does not say anything on the effective possibility to learn in an easy way the parameters of the network!

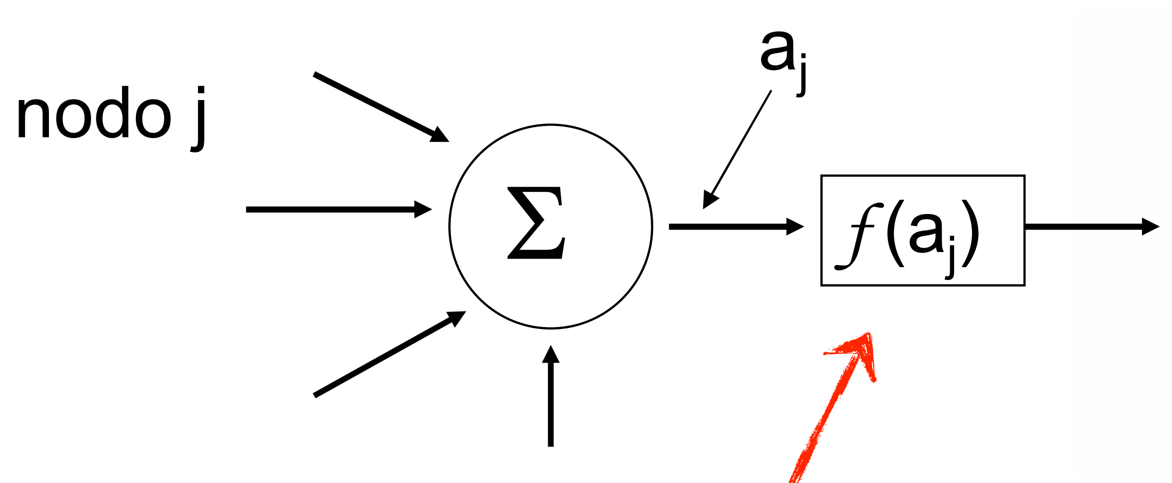
FEED-FORWARD ANN

- the most used ANN have a Feed-Forward multilayer structure:

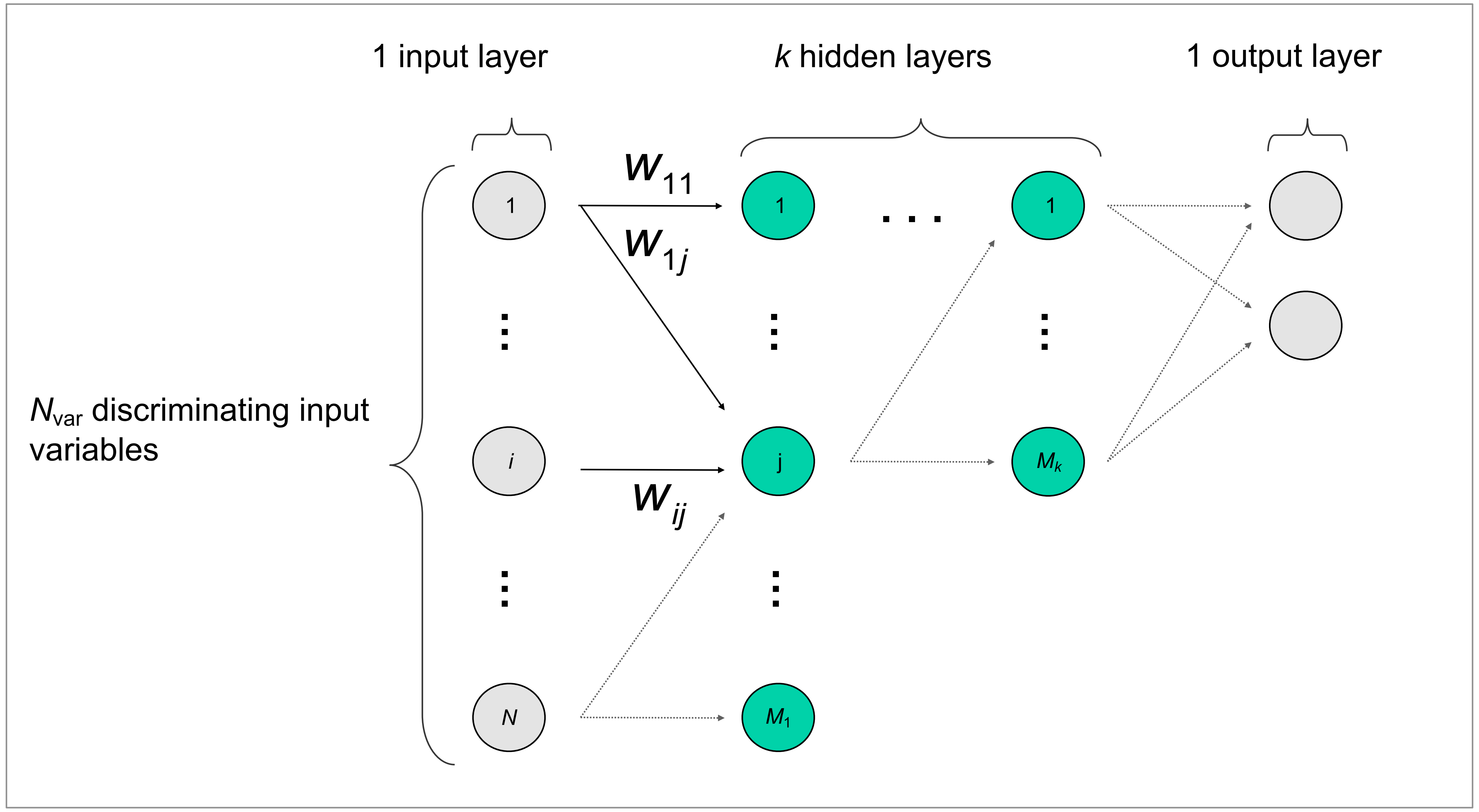


- neurons organised in layers: input, hidden-1, ... , hidden-K, output
- only connections from a given layer to the next following one are allowed

Nodo



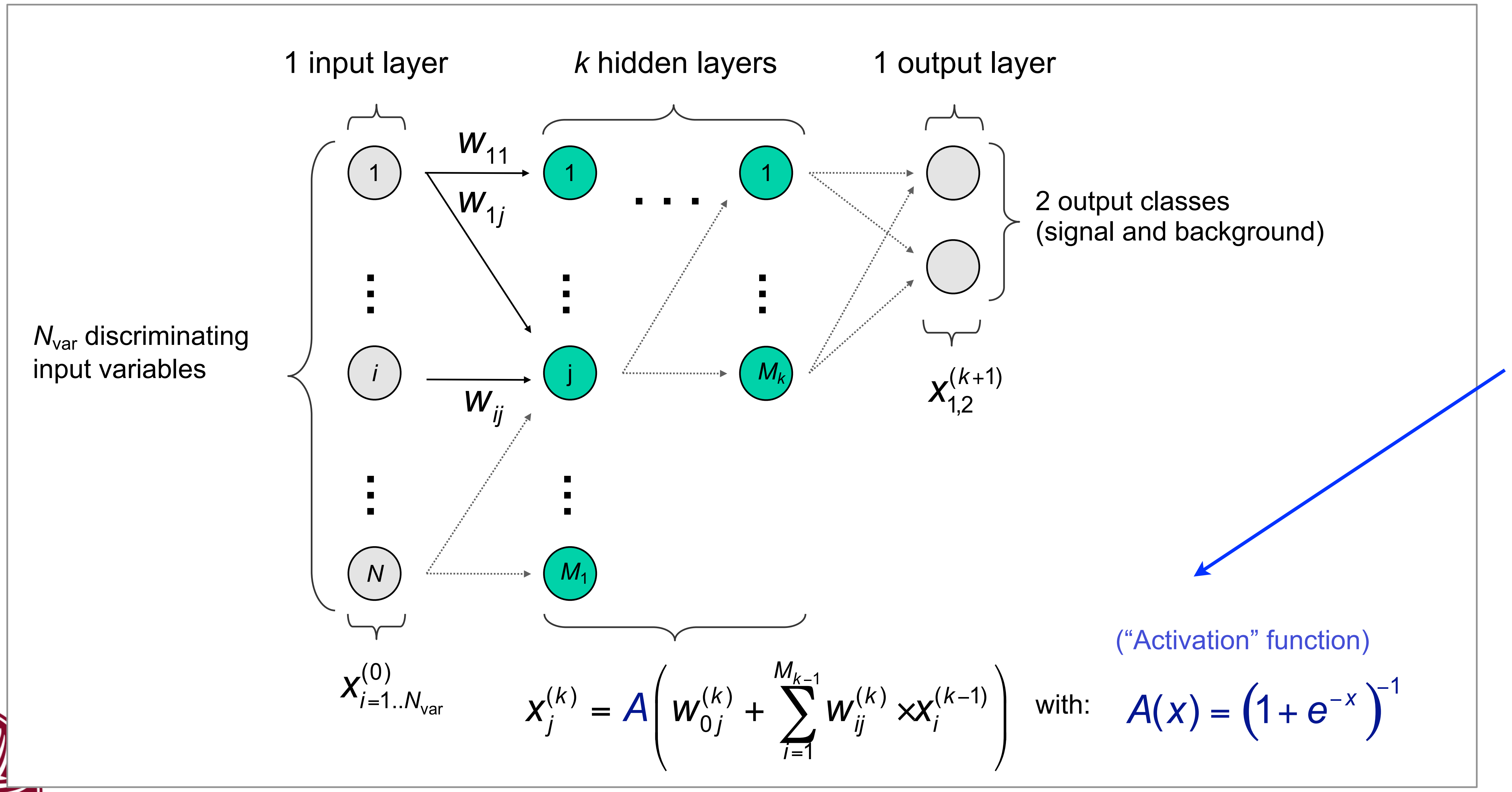
activation function (or output function)

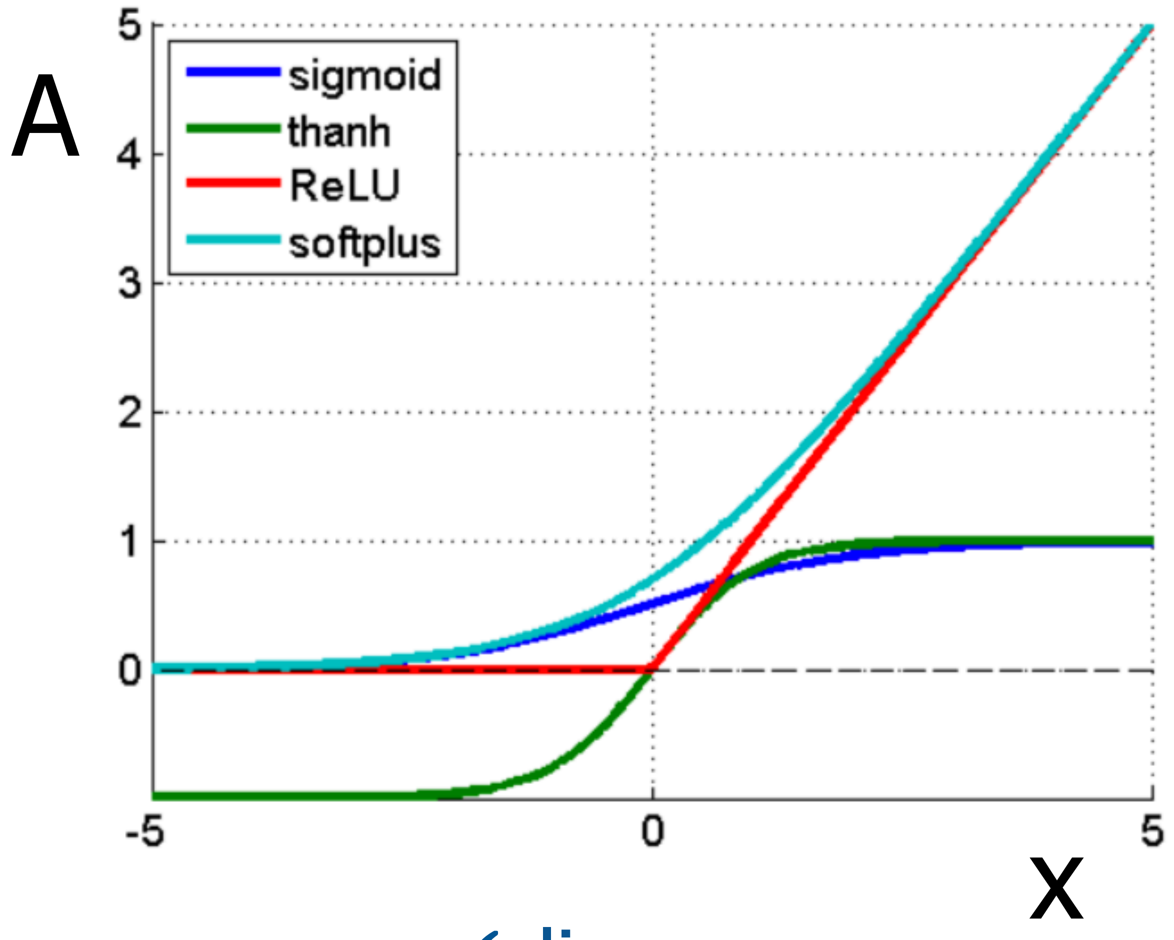


Feed-forward Multilayer Perceptron

RESPONSE FUNCTION

- behaviour of the NN determined by:
  - topological structure of the neurons (architecture)
  - Weights associated to each connection
  - response function of each neutron to the input data
- Response function ρ:
  - maps the input of the neuro n:$x^{(k-1)}{}_1,\ldots,x^{(k-1)}{}_n$ to the output $x^{(k)}{}_j$
  - normally divided in two parts: synaptic function $k:R^n \rightarrow R$ and the neural activation function $A:R \rightarrow R$: $\rho = k \bullet A$





$$A : x \rightarrow \begin{cases} \text{linear: } x \\ \text{sigmoid: } 1/(1+e^{x}) \\ \text{Tanh}(x) \\ \text{ReLU: } \max(0,x) \\ \text{softplus: } \log(1+e^{x}) \end{cases}$$

TRAINING

- The training of the NN consists in adjusting the weights (and the other hyperparameters) according to a given loss function in order to optimise the performance of the algorithm wrt a specific task
- most used technique: Back-propagation

Output for an ANN with:
- a single hidden layer with A: tanh
- an output layer with A: linear

n_h: number of hidden layer neurons

n_{var}: number of input layer neurons

$$y_{ANN} = \sum_{j=1}^{n_h} x_j^{(2)} w_{j1}^{(2)} = \sum_{j=1}^{n_h} \tanh\left(\sum_{i=1}^{n_{var}} x_i w_{ij}^{(1)}\right) w_{j1}^{(2)}$$

weight associated to the link between j-th neuron of the hidden layer and the output neutron

weight associated to the link between the i-th neuron of the input layer and the j-th neuron of the hidden layer

TRAINING

- during the training N examples are presented to the NN: $\boldsymbol{x}_a$ (a=1,..,N)
- for each event the output $y_{ANN}(a)$ is computed and compared with the expected target $Y_a \in \{0,1\}$ (0 class 2, 1 class 1 as example for a 2-class classification algorithm)
- A loss function is defined in order to measure the distance between $y_{ANN}(a)$ e Y_a:

$$\Delta(x_1, ..., x_N|\mathbf{w}) = \sum_{\mathbf{a=1}}^{\mathbf{N}} \boldsymbol{\Delta}_{\mathbf{a}}(\mathbf{x}_{\mathbf{a}}|\mathbf{w}) = \sum_{\mathbf{a=1}}^{\mathbf{N}} \frac{\mathbf{1}}{\mathbf{2}}(\mathbf{y}_{\mathbf{ANN}}(\mathbf{a}) - \mathbf{Y}_{\mathbf{a}})^{\mathbf{2}}$$

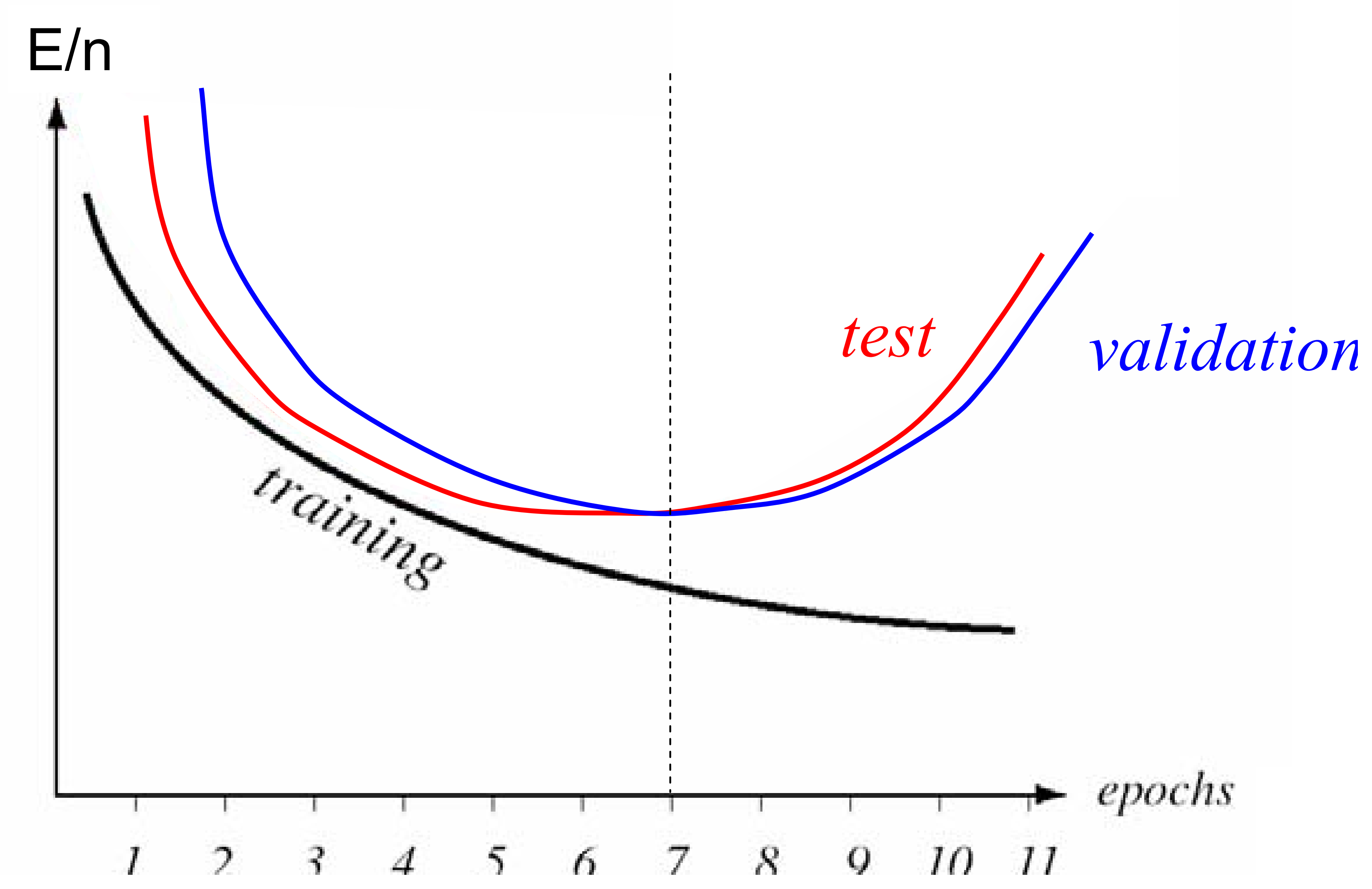
MSE

- and the weight vector is chosen as the one that minimise the error Δ
  - Minimisation obtained with the GD/SGD ...

$$\mathbf{w}^{(\rho+\mathbf{1})} = \mathbf{w}^{(\rho)} - \eta \nabla_{\mathbf{w}} \boldsymbol{\Delta}$$

LEARNING CURVES

- at the start of the training phase the error on the training set is typically large
- with the iterations (epochs) the error tend to decrease until it reach a plateau value that depends on:
    - training set size
    - number of weights of the NN
    - initial value of the weights
- training progress is visualized with the learnign curve (error vs epochs)
- as usual multiple datasets (or cross validation) are needed to train the NN, decide the architecture, decide the stop criterion, and evaluate the final performances … etc..

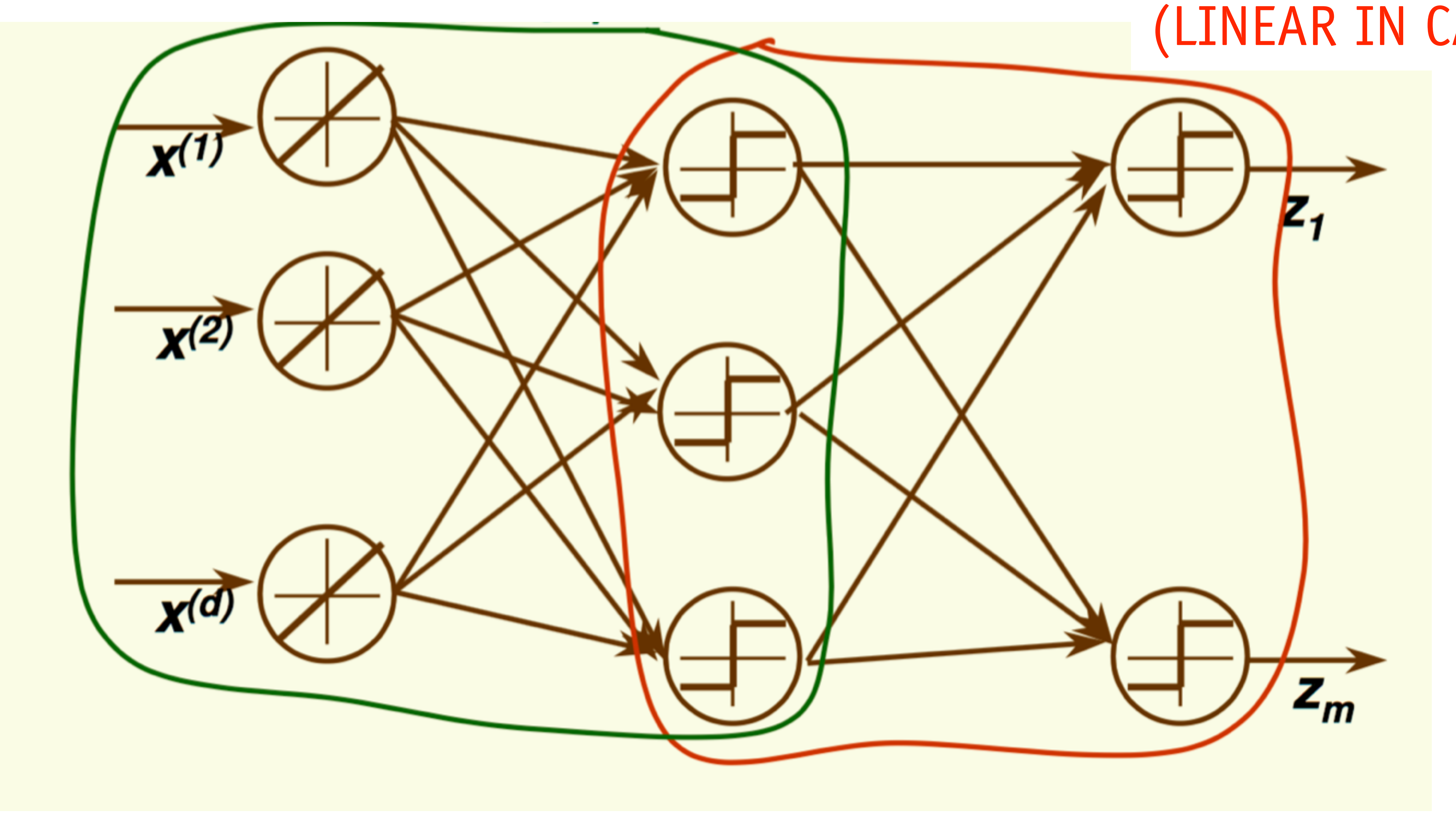


ANN: INTERPRETATION AS NON LINEAR MAPPING

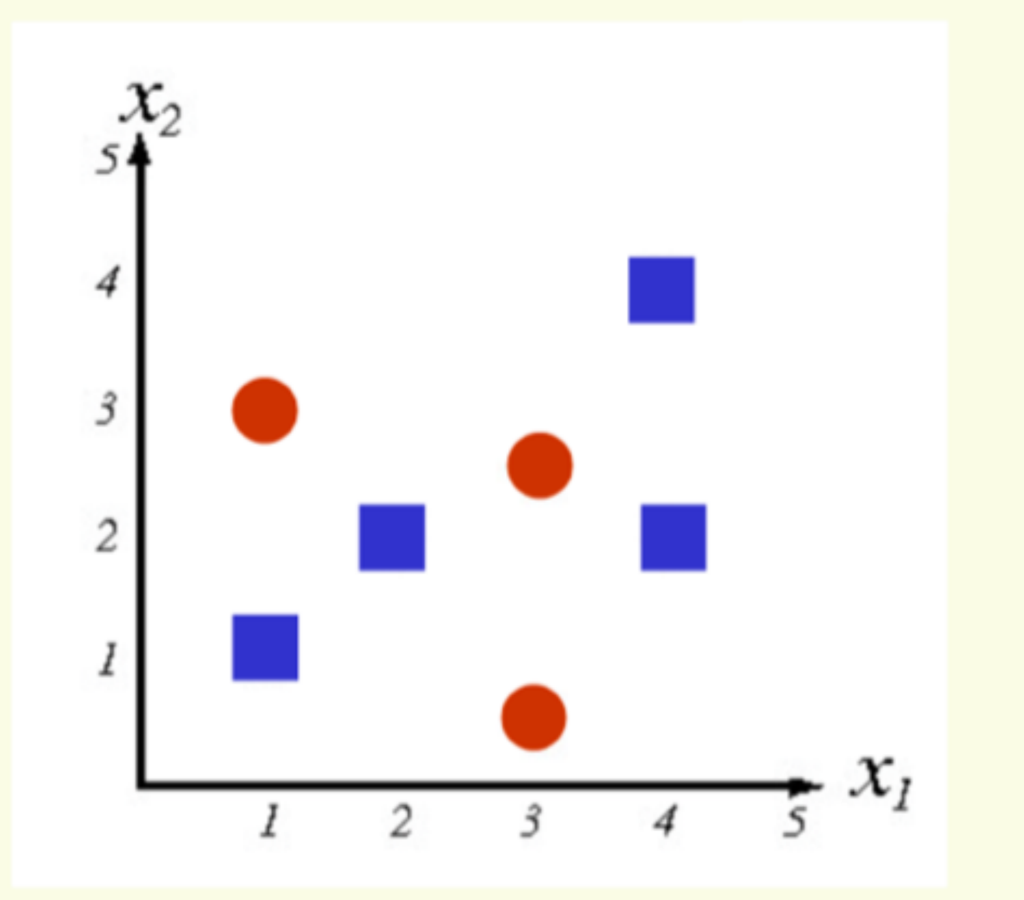
- A NN can be thought as an algorithm that learn two tasks at the same time:

THIS MODULE LEARN A (NON LINEAR) MAPPING
OF THE INPUT

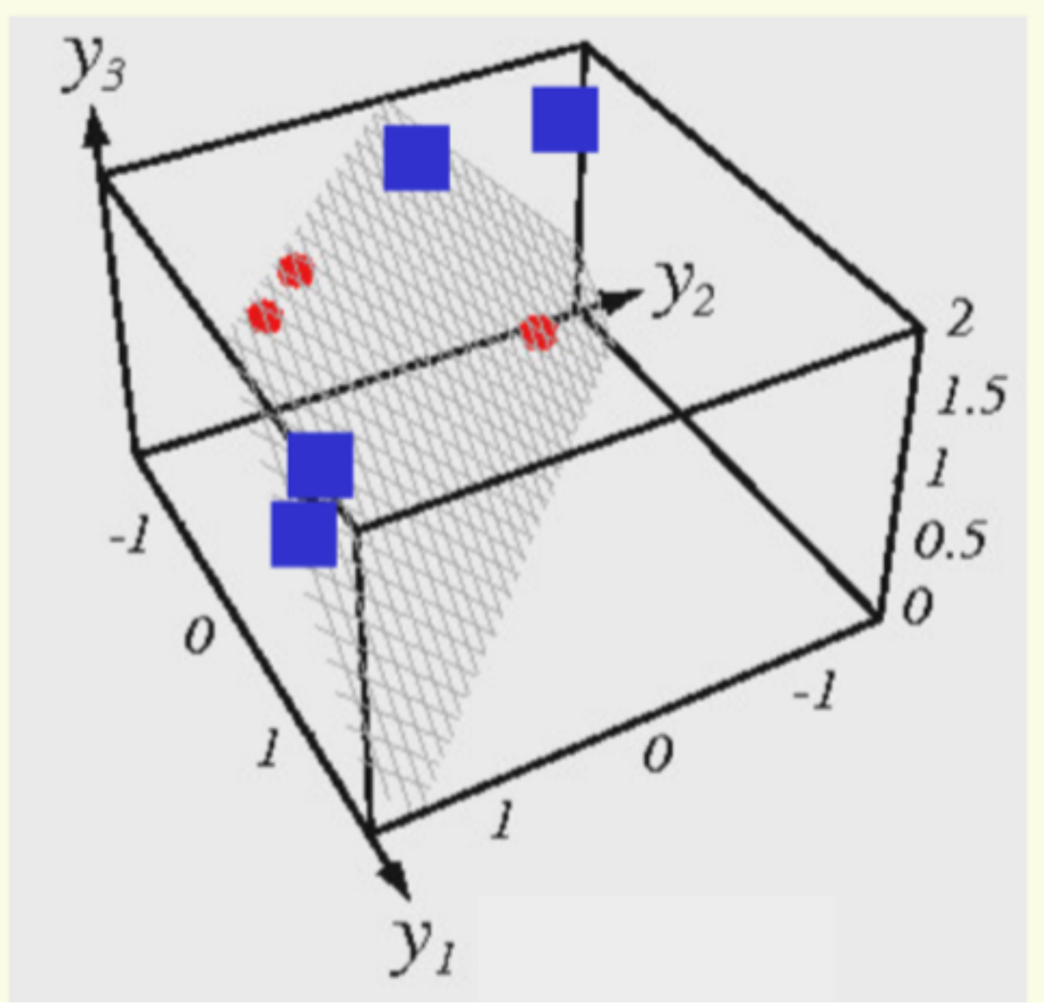
THIS MODULE LEARN A CLASSIFIER
(LINEAR IN CASE OF A PERCEPTRON)



original space:
non linearly separable patterns x:

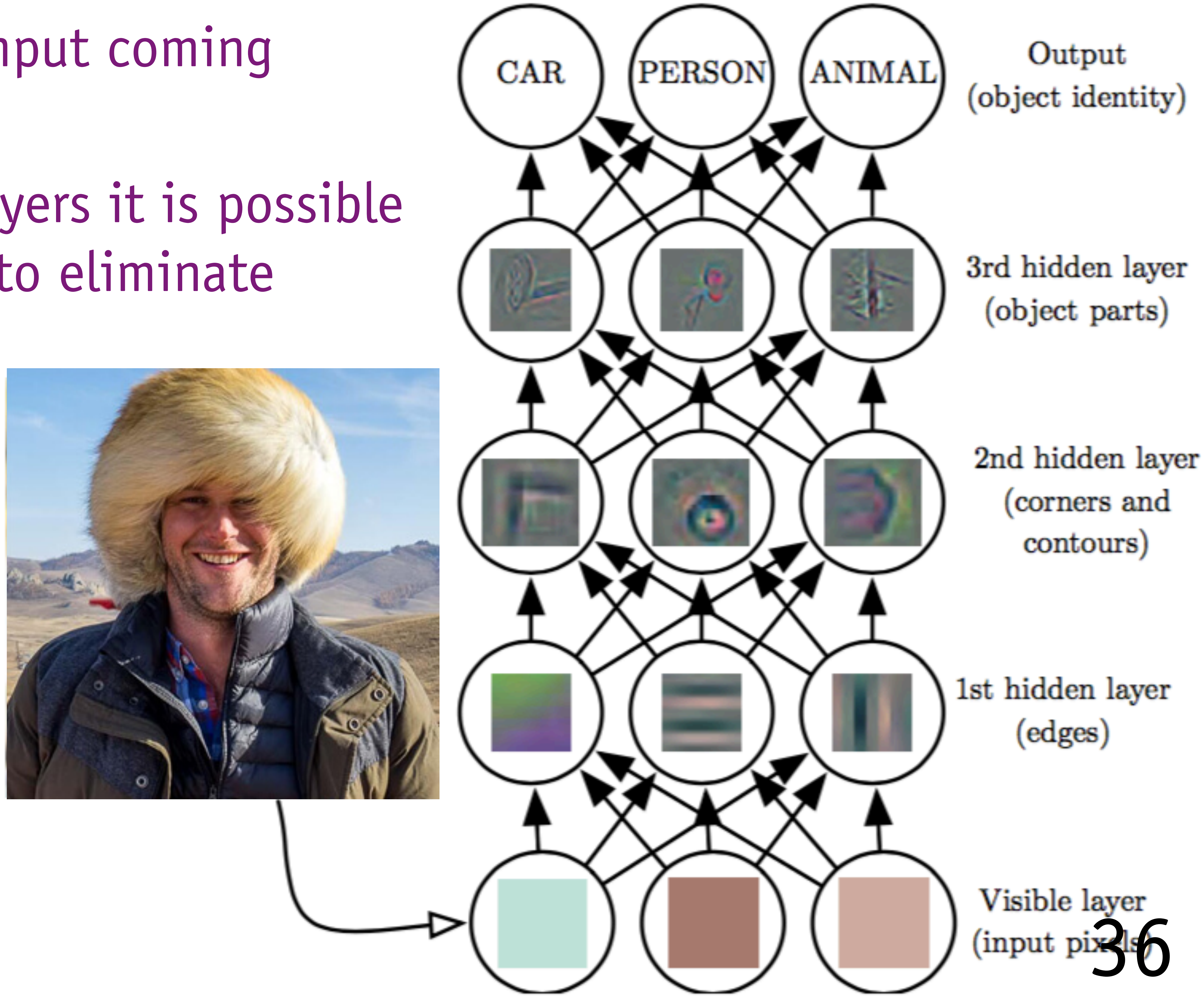


NN: finds the non linear mapping $y=\Phi(x)$ in 3-dimensional space (three hidden nodes) in which the patterns are linearly separable

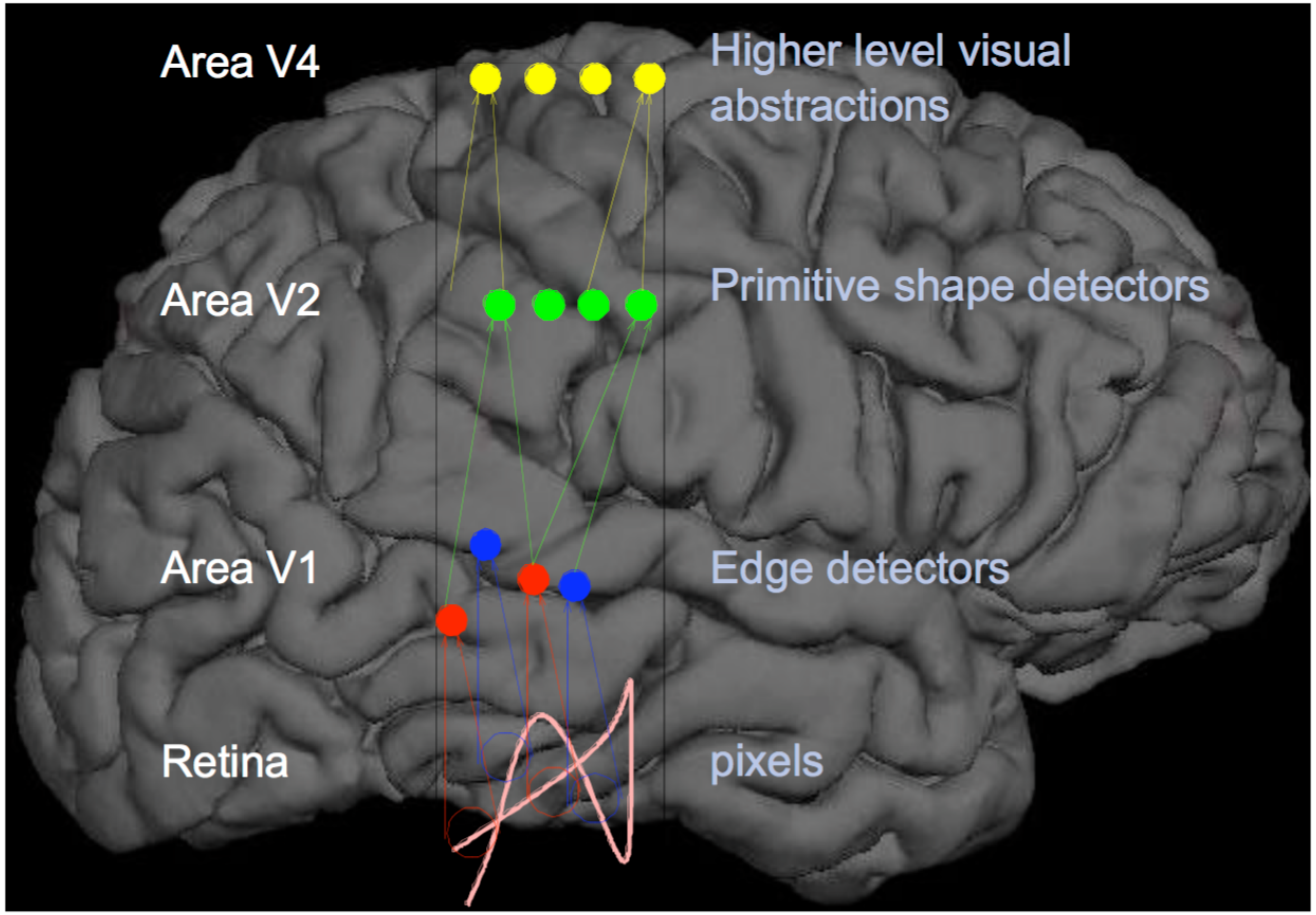


DEEP LEARNING AND ANN

- the different transformation/representation layers have a natural and intuitive implementation in multilayer neural-networks:
- each layer implements a transformation of the input coming from the preceding layer
- by using a sufficiently large number of hidden layers it is possible to learn extremely complex representations and to eliminate from the process irrilevante variations
  - example: image → array of raw pixels
  - first layer: find presence/absence of strong tonal Variations in specific points of the image (edges)
  - second layer: combines edges to find patterns like corners, contours
  - third layer: combines the previous patterns in complex objects (like faces, heads, …) that can be used to classify the content of the image …



DEEP ARCHITECTURE OF THE BRAIN



- we organise ideas and concept in hierarchical way
- first we learn simple concepts, then we compose them to represent more abstract concepts
- the DL try to emulate this behaviour …