# Artificial Neural Networks: Lecture 3

## Statistical classification by deep networks

Wulfram Gerstner

EPFL, Lausanne, Switzerland

**Objectives for today:**

- The cross-entropy error is the optimal loss function for classification tasks
- The sigmoidal (softmax) is the optimal output unit for classification tasks
- Multi-class problems and '1-hot coding'
- Under certain conditions we may interpret the output as a probability
- The rectified linear unit (RELU) for hidden layers

# Reading for this lecture:

**Bishop 2006**, Ch. 4.2 and 4.3

*Pattern recognition and Machine Learning*

or

**Bishop 1995**, Ch. 6.7 – 6.9

*Neural networks for pattern recognition*

**or**

**Goodfellow et al.,2016** Ch. 5.5, 6.2, and 3.13 of

*Deep Learning*

Miniproject1: soon!

**You will work with**

- regularization methods (see last week)
- cross-entropy error function
- sigmoidal (softmax) output
- rectified linear hidden units
- 1-hot coding for multiclass

This week

- batch normalization
- Adam optimizer

Next week

# Review: Data base for Supervised learning (single output)

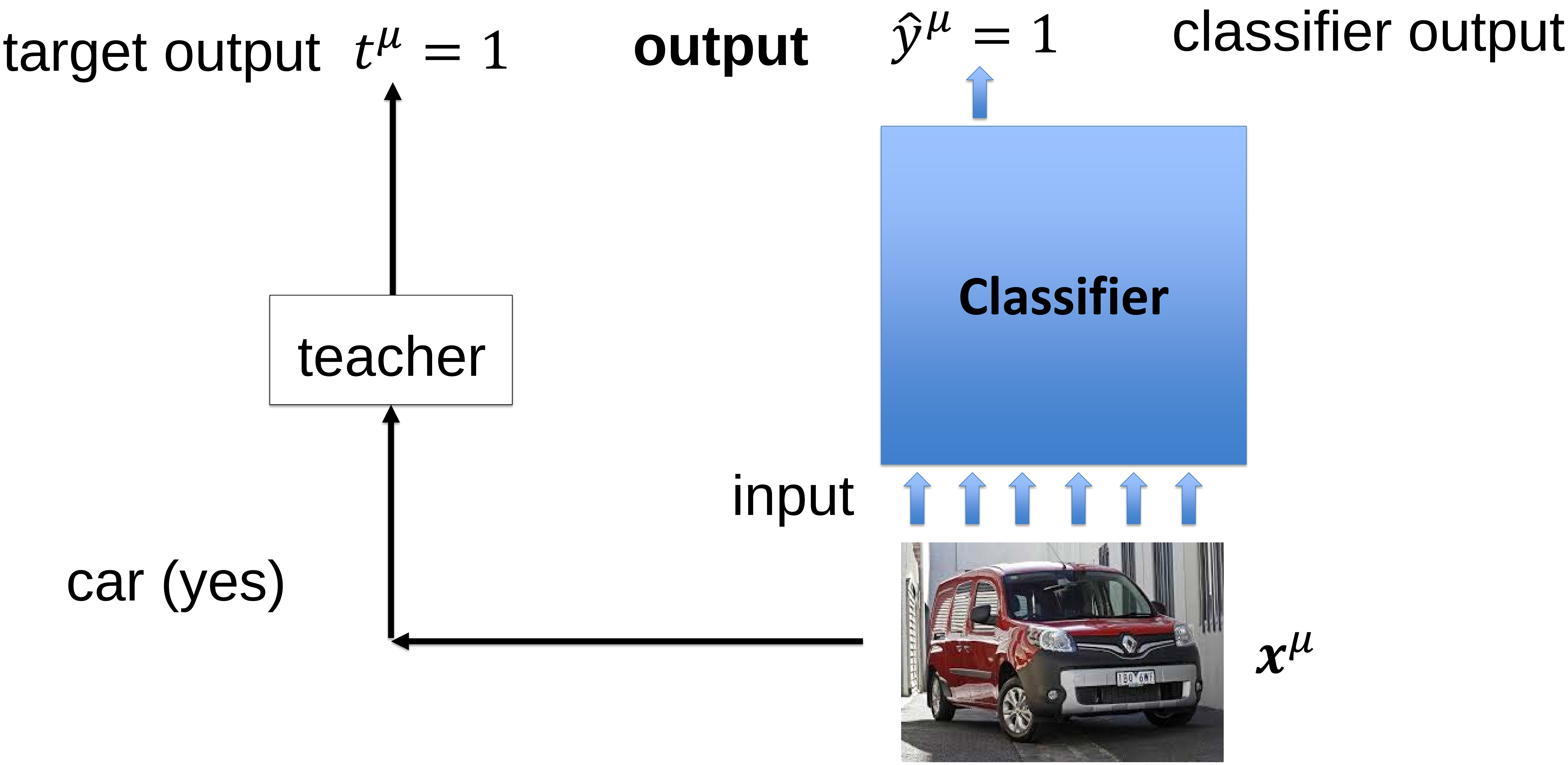
$P$ data points $\{ \quad (\boldsymbol{x}^\mu, t^\mu) \quad , \qquad 1 \le \mu \le P \quad \};$

input target output

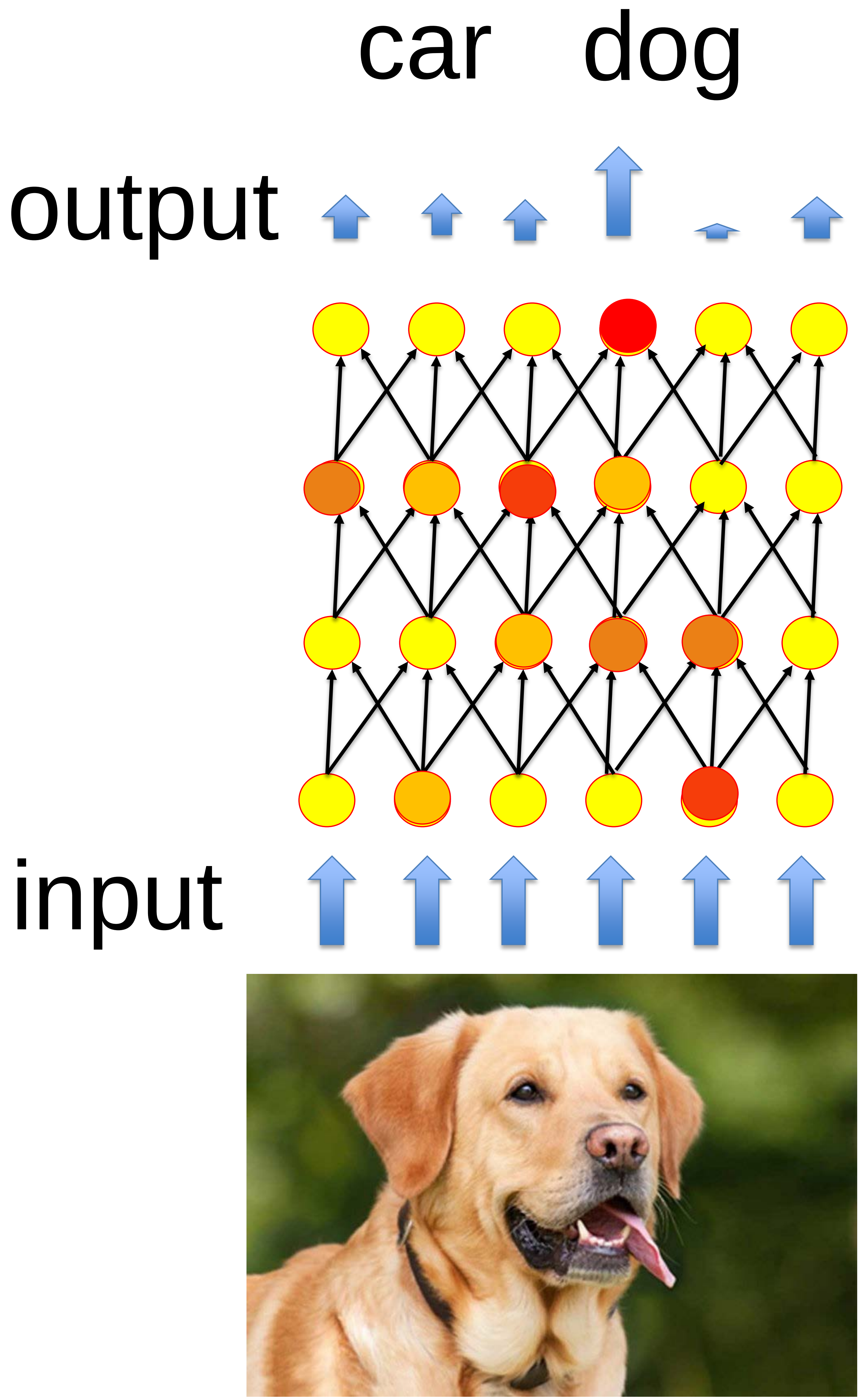
$t^\mu = 1$ car =yes

$t^\mu = 0$ car =no

# review: Supervised learning

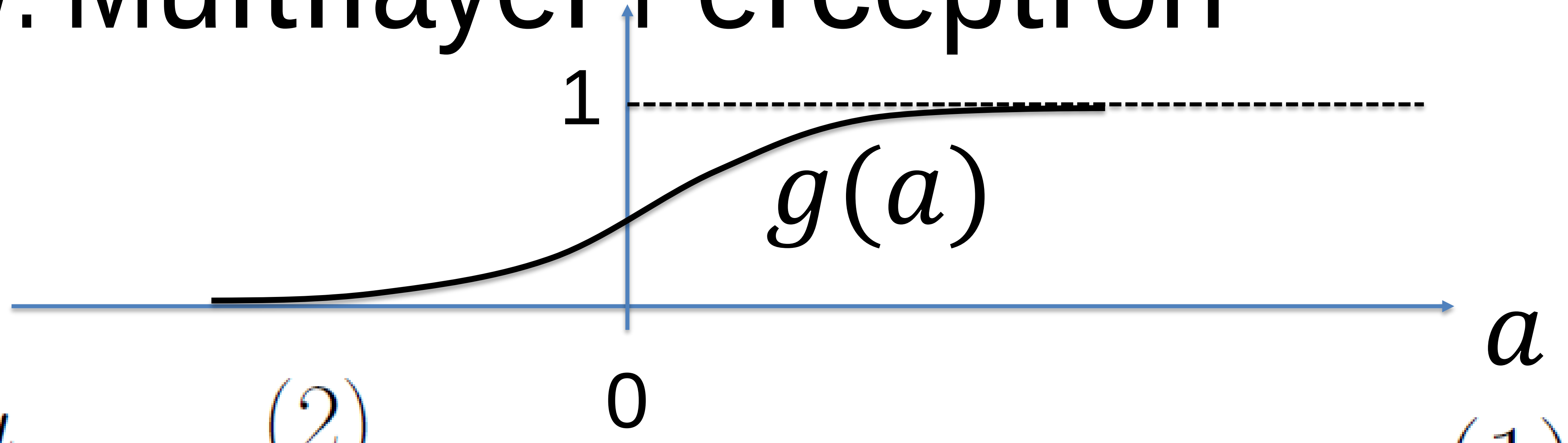


# review: Artificial Neural Networks for classification




**Aim of learning:**
Adjust connections such that output is correct (for each input image, **even new ones**)

# Review: Multilayer Perceptron



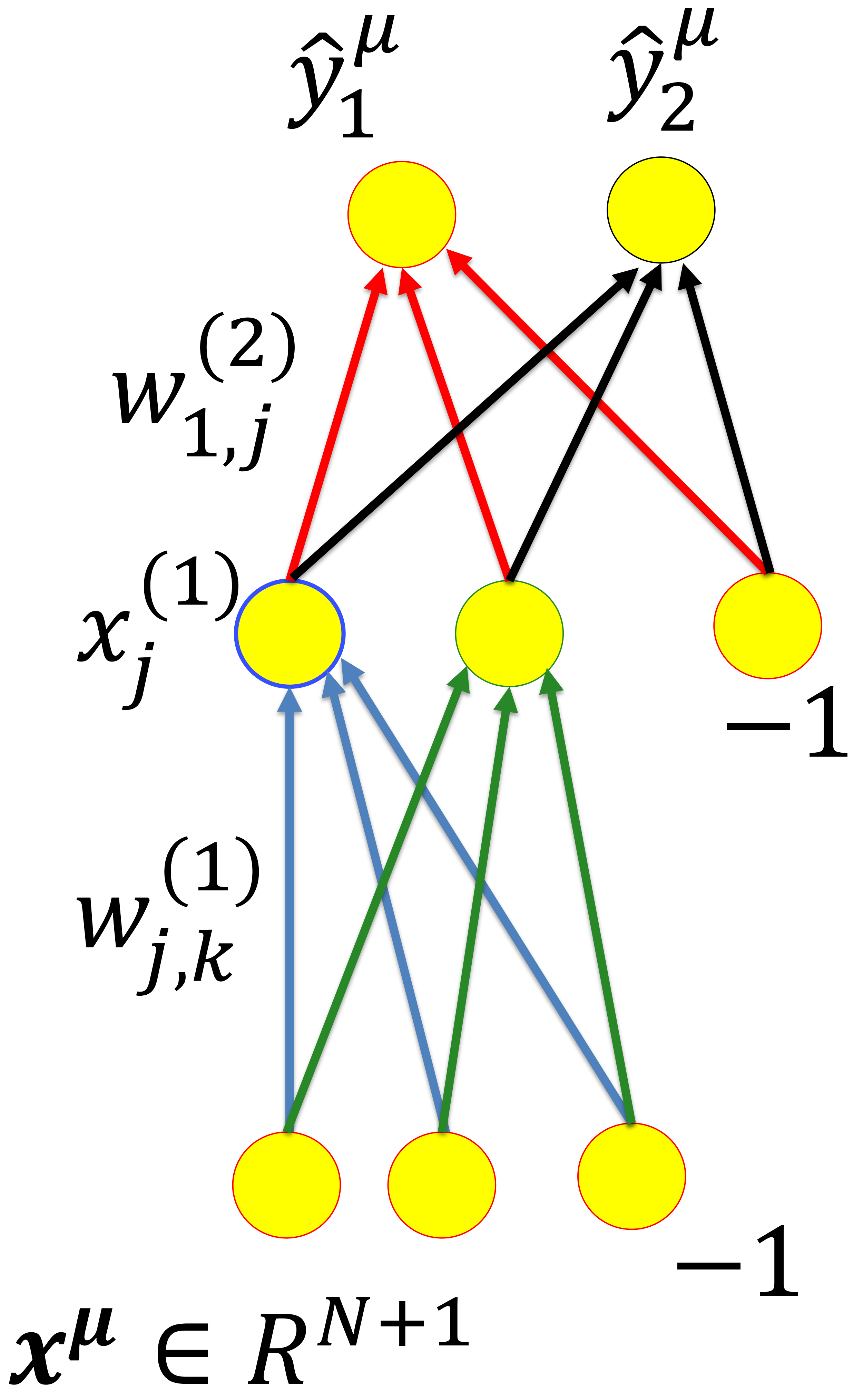

$$\hat{y}_i^{\mu} = x_i^{(2)} \quad (1)$$

$$= g^{(2)}[a_i^{(2)}] \quad (2)$$

$$= g^{(2)}[\sum_j w_{ij}^{(2)} x_j^{(1)}] \quad (3)$$

$$= g^{(2)}[\sum_j w_{ij}^{(2)} g^{(1)}(a_j^{(1)})] \quad (4)$$

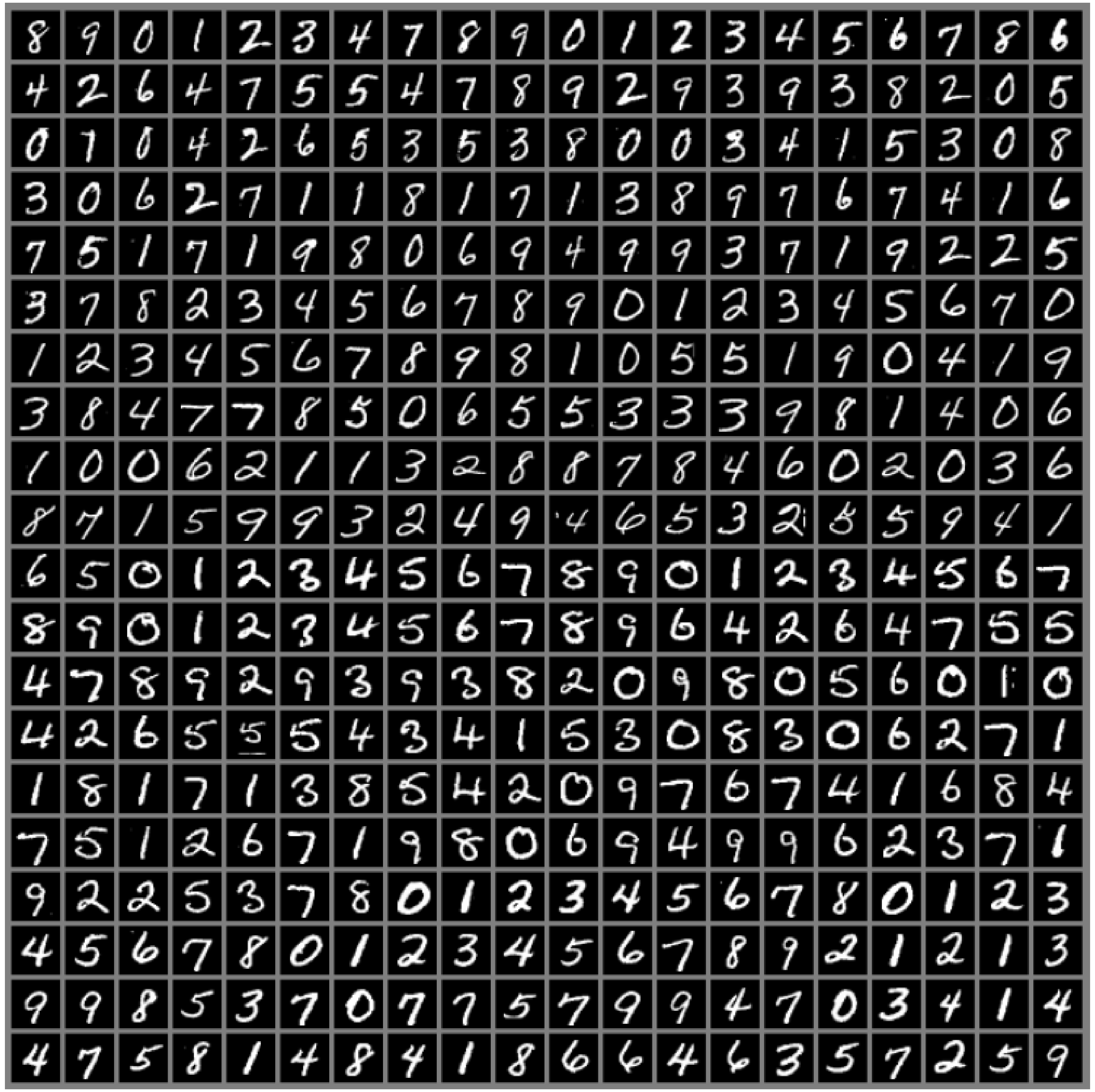
$$= g^{(2)}[\sum_j w_{ij}^{(2)} g^{(1)}(\sum_k w_{jk}^{(1)} x_k^{\mu})] \quad (5)$$



# Review: Example MNIST

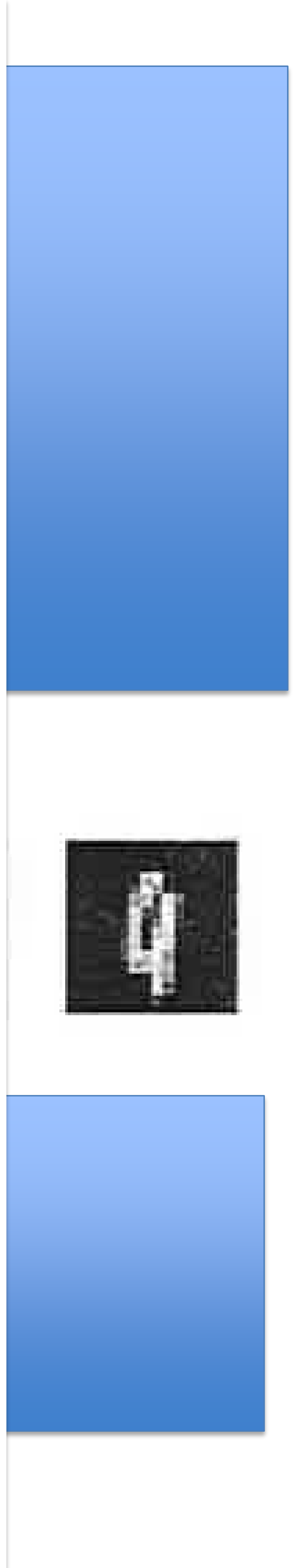
- images 28x28
- Labels: 0, …, 9
- 250 writers
- 60 000 images in training set

MNIST data samples



*Picture: Goodfellow et al, 2016*
*Data base:*
*http://yann.lecun.com/exdb/mnist/*

# review: data base is noisy



9 or 4?

9 or 4?

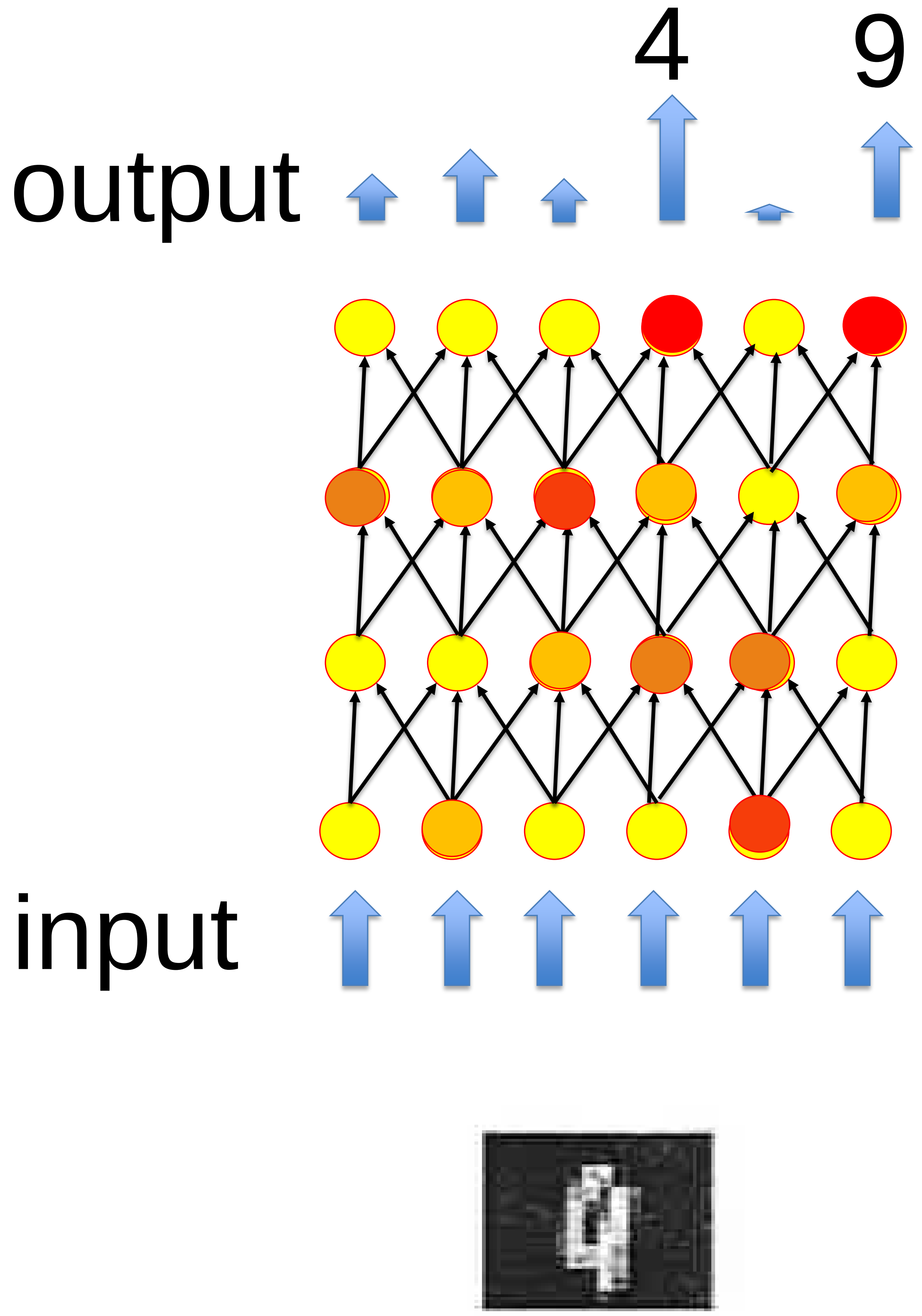
- training data is always noisy
- the future data has different noise

- Classifier must extract the essence
  → **do not fit the noise!!**

What might be a
9 for reader A
Might be a
4 for reader B

# Question for today

May we interpret the outputs our network as a probability?



# Artificial Neural Networks: Lecture 3

## Statistical Classification by Deep Networks

Wulfram Gerstner
EPFL, Lausanne, Switzerland

1. The statistical view: generative model

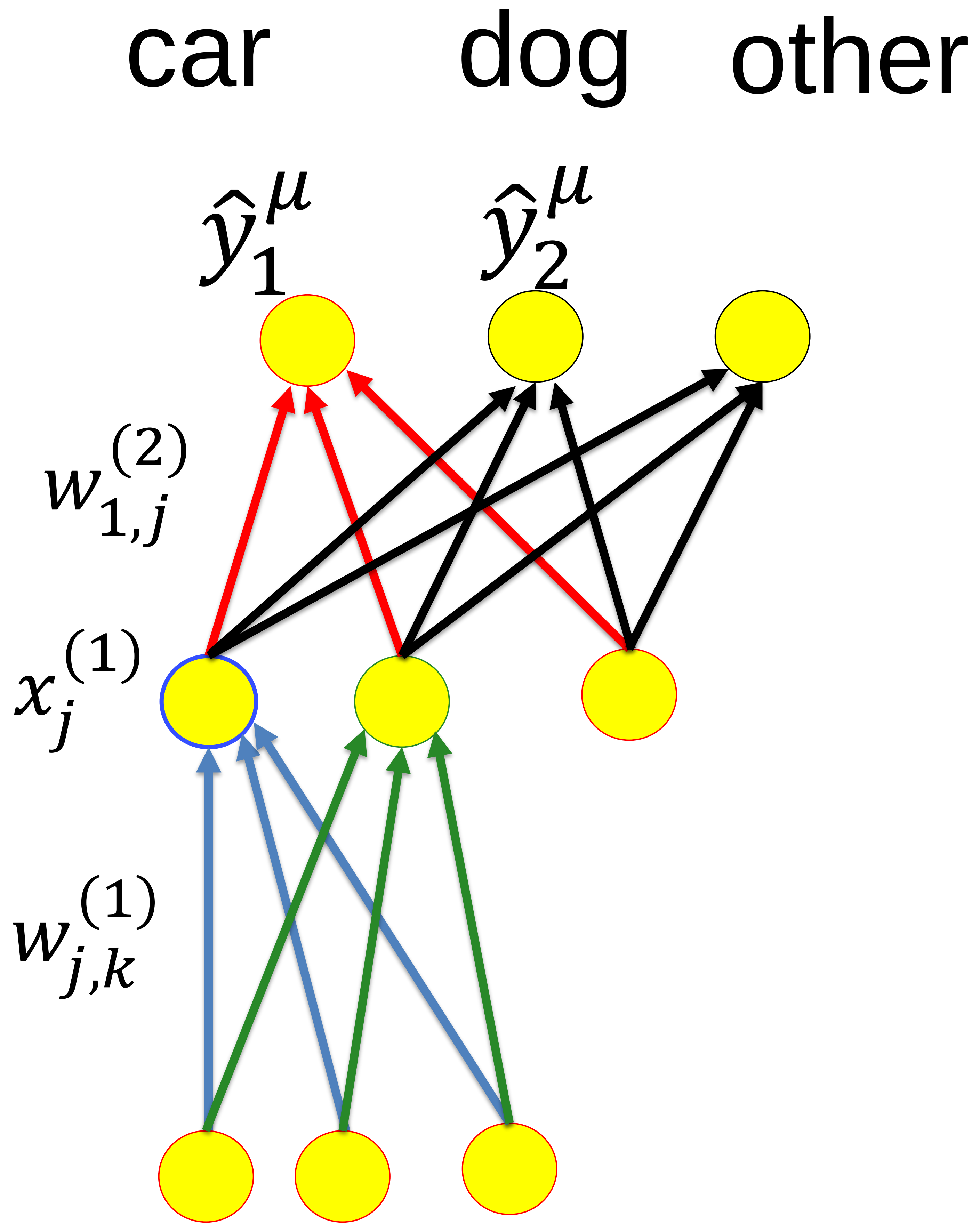
# 1. The statistical view

**Idea:**

interpret the output $\hat{y}_k^{\mu}$
as the **probability** that
the novel input pattern $\boldsymbol{x}^{\boldsymbol{\mu}}$
should be classified
as class $k$

$\hat{y}_k^{\boldsymbol{\mu}} = \mathrm{P}(C_k|\boldsymbol{x}^{\boldsymbol{\mu}})$ pattern from data base

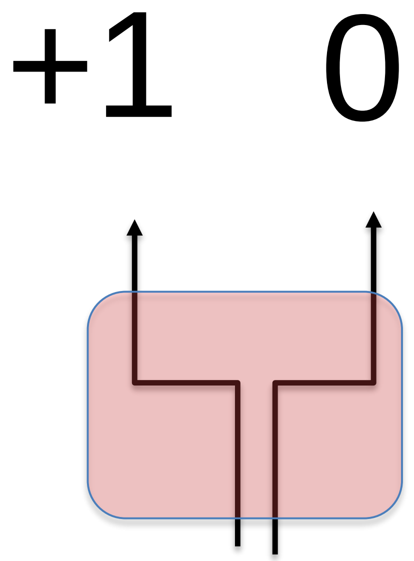
$\hat{y}_k = \mathrm{P}(C_k|\boldsymbol{x}\ \ )$ arbitrary novel pattern




$\boldsymbol{x}^{\boldsymbol{\mu}} \in R^{N+1}$

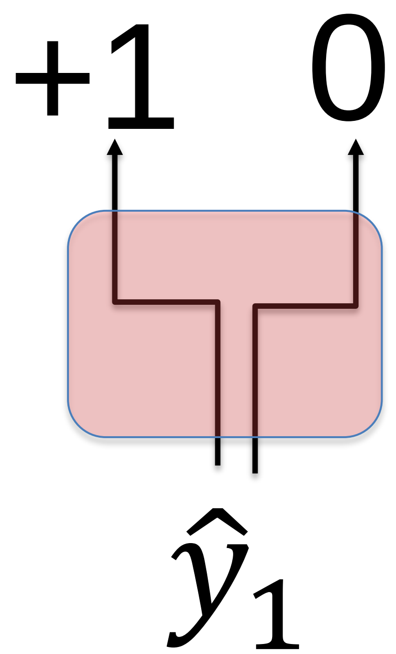
# 1. The statistical view: single class

$p_+ = \hat{y}_1$



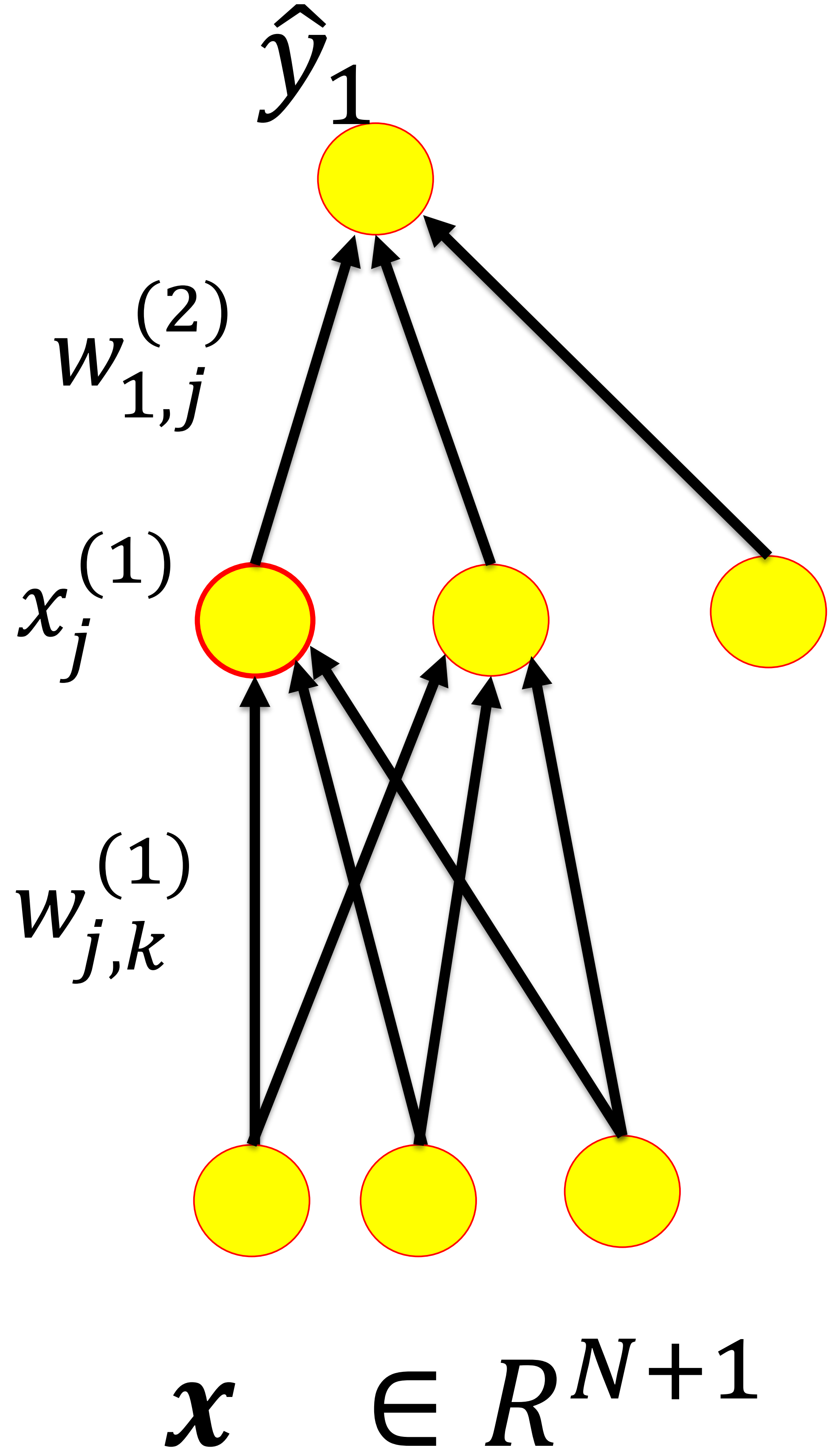

$p_- = 1 - \hat{y}_1$

Take the output $\hat{y}_1$ and generate predicted labels $\hat{t}_1$ probabilistically




→ generative model for class label with $\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$

predicted label



# Artificial Neural Networks: Lecture 3
# Statistical Classification by Deep Networks

Wulfram Gerstner
EPFL, Lausanne, Switzerland

1. The statistical view: generative model
2. **The likelihood of data under a model**

# 2. The likelihood of a model (given data)

Overall aim:

What is the probability that my set of $P$ data points

$$\{ \quad (\boldsymbol{x}^\mu, t^\mu) \quad , \qquad 1 \leq \mu \leq P \quad \};$$

**could have been generated** by my model?

# 2. The likelihood of a model

Detour:

forget about labeled data, and just think of input patterns

What is the probability that a set of $P$ data points

$$\left\{ \boldsymbol{x}^k ; 1 \leq \mathrm{k} \leq P \right\};$$

**could have been generated** by my model?

# 2. Example: Gaussian distribution

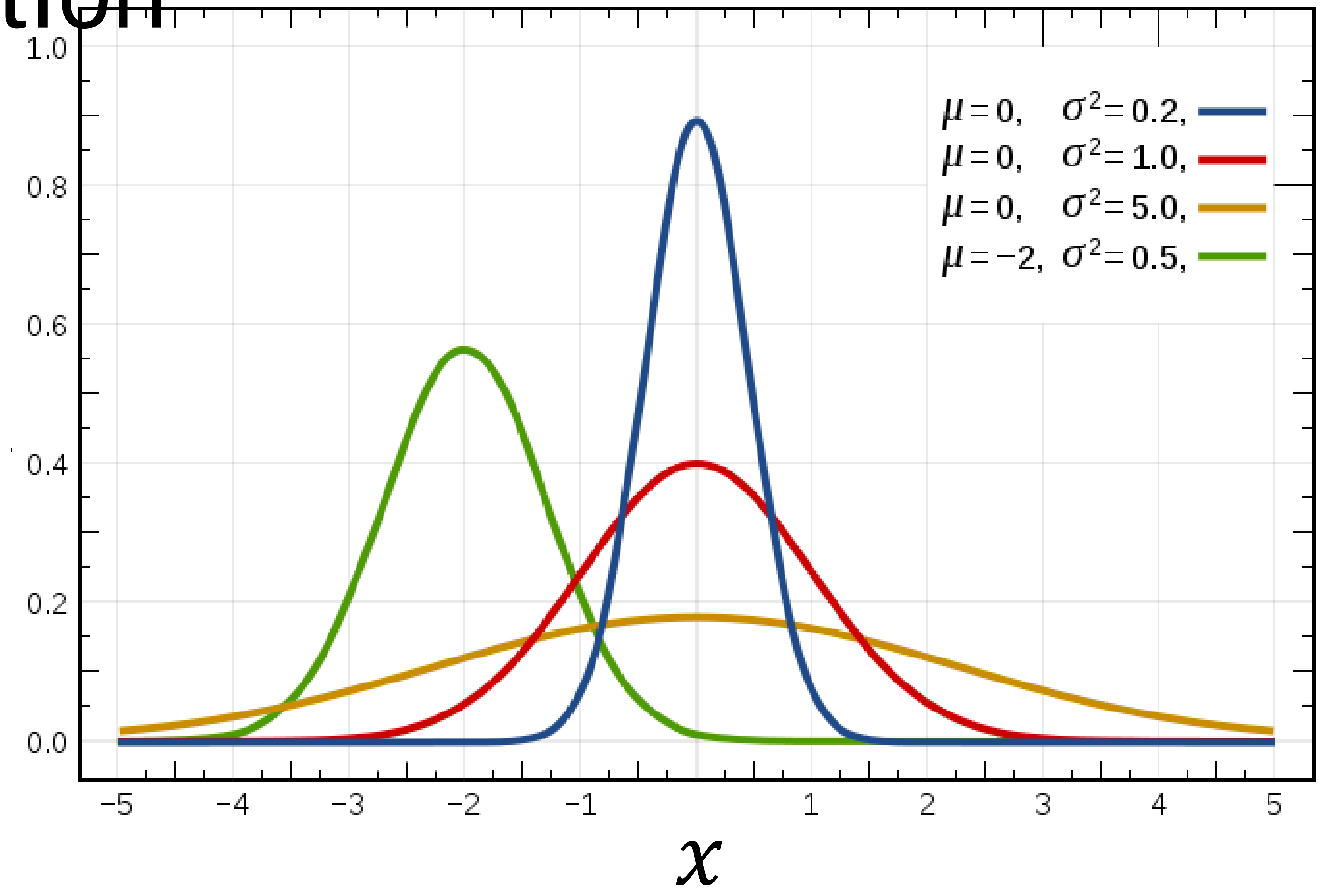
$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} exp\left\{\frac{-(x-\mu)^2}{2\sigma^2}\right\}_1$$

this depends on 2 parameters

$$\{w_{1,} w_{2,}\} = \{\mu, \sigma\}$$

center

width

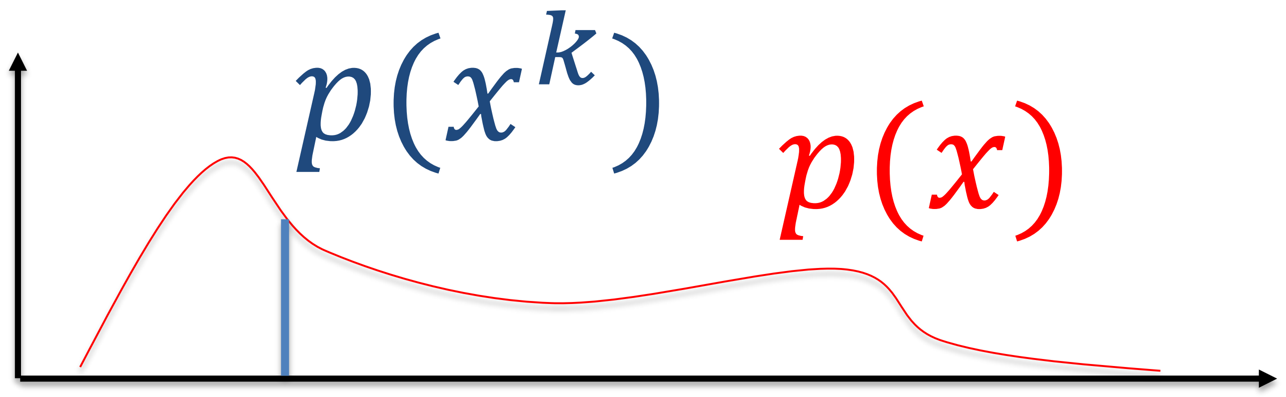



https://en.wikipedia.org/wiki/Gaussian_function#/media/

# 2. Random Data Generation Process

Probability that a random data generation process draws one sample $k$ with value $x^k$ is

$$\sim p(x^k)$$




**Example**: for the specific case of the Gaussian

$$p(x^k) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{\frac{-(x^k-\mu)^2}{2\sigma^2}\right\}$$

What is the probability to generate P data points?

*Blackboard 1:*

generate P data points

# 2. Likelihood function (beyond Gaussian)

Suppose the probability for generating a data point $\boldsymbol{x}^k$ using my model is proportional to

$$p(\boldsymbol{x}^k)$$

Suppose that data points are generated independently.

Then the likelihood that **my actual data** set

$$\boldsymbol{X} = \{\boldsymbol{x}^k; 1 \leq k \leq P \quad \};$$

**could have been generated** by my model is

$$p_{model}(\boldsymbol{X}) = \; p(\boldsymbol{x}^1)\, p(\boldsymbol{x}^2)\, p(\boldsymbol{x}^3) \ldots p(\boldsymbol{x}^P)$$

# 2. Maximum Likelihood (beyond Gaussian)

$$p_{model}(\boldsymbol{X}) = \quad p(\boldsymbol{x}^1)\, p(\boldsymbol{x}^2)\, p(\boldsymbol{x}^3) \dots p(\boldsymbol{x}^P)$$

BUT this likelihood depends on the parameters of my model

$$p_{model}(\boldsymbol{X}) = p_{model}\left(\boldsymbol{X} \middle| \{w_1, w_2, \dots w_n,\}\right)$$

parameters

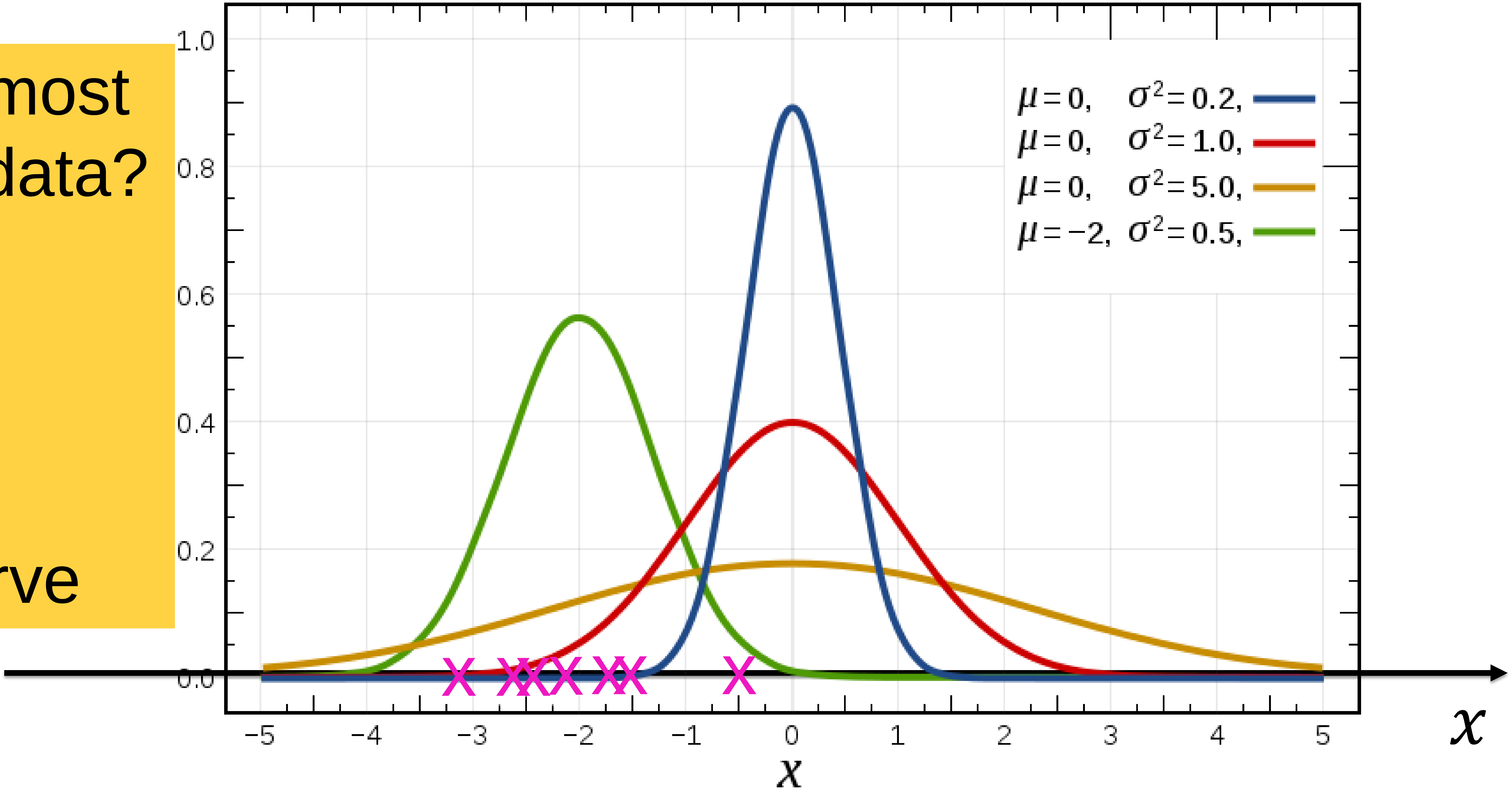
Choose the parameters such that the likelihood is maximal!

# 2. Example: Gaussian distribution

Likelihood of point $x^k$ is $p(x^k) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{\frac{-(x^k-\mu)^2}{2\sigma^2}\right\}$

Which Gaussian is most consistent with the data?

[ ] green curve
[ ] blue curve
[ ] red curve
[ ] brown-orange curve



# 2. Example: Gaussian

$$p_{model}(\boldsymbol{X}) = \quad p(\boldsymbol{x}^1)\, p(\boldsymbol{x}^2)\, p(\boldsymbol{x}^3) \ldots p(\boldsymbol{x}^P)$$

The likelihood depends on the 2 parameters of my Gaussian

$$p_{model}(\boldsymbol{X}) = p_{model}\left(\boldsymbol{X} \middle| \{w_1, w_2\}\right)$$

$$p_{model}(\boldsymbol{X}) = p_{model}(\boldsymbol{X}|\{\mu, \sigma\})$$

Exercise 1 NOW! (8 minutes): you have $P$ data points
Calculate the **optimal choice** of parameter $\mu$:
To do so maximize $p_{model}(\boldsymbol{X})$ with respect to $\mu$

*Blackboard 2:*

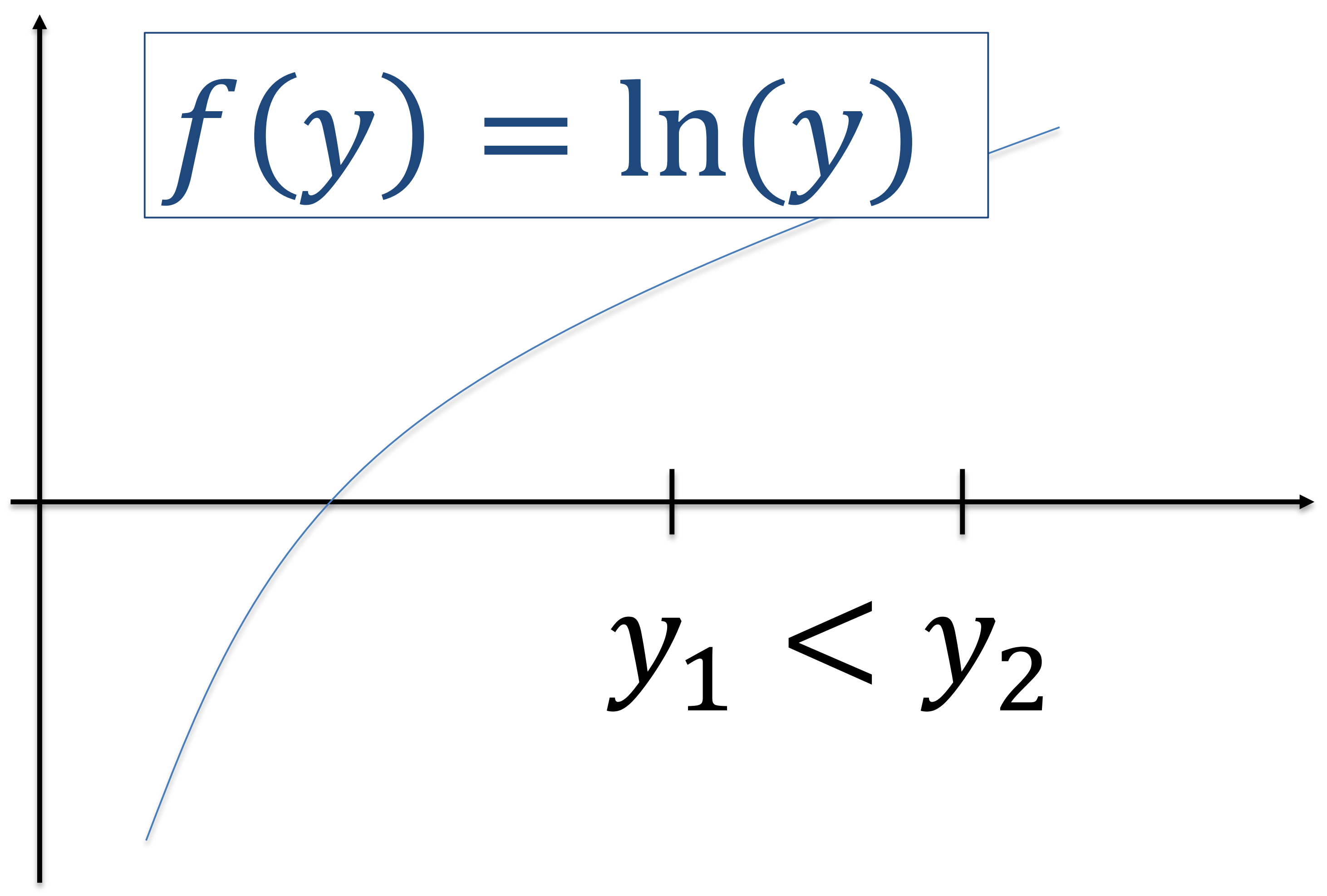
Gaussian: best parameter choice for center

# 2. Maximum Likelihood (general)

Choose the parameters such that the likelihood

$$p_{model}(\boldsymbol{X}|\{w_{1,}w_{2,}\ldots w_{n,}\}) = p(\boldsymbol{x}^1)\, p(\boldsymbol{x}^2)\, p(\boldsymbol{x}^3) \ldots p(\boldsymbol{x}^P)$$

is maximal




Note:
Instead of maximizing

$$p_{model}(\boldsymbol{X}|param)$$

you can also maximize

$$\ln(p_{model}(\boldsymbol{X}|param))$$

# 2. Maximum Likelihood (general)

Choosing the parameters such that the likelihood

$$p_{model}\left(\boldsymbol{X}|\{w_1, w_2, \dots w_n\}\right) = p(\boldsymbol{x}^1)\, p(\boldsymbol{x}^2)\, p(\boldsymbol{x}^3) \dots p(\boldsymbol{x}^P)$$

is maximal is equivalent to maximizing the log-likelihood

$$LL(\{w_1, w_2, \dots w_n\}) = \ln(p_{model}) = \sum_k ln\, p(\boldsymbol{x}^k)$$

**“Maximize the likelihood that the given data could have been generated by your model”**
(even though you know that the data points were generated by a process in the real world that might be very different)

# 2. Maximum Likelihood (general)

Choose the parameters such that the likelihood

$$p_{model}\left(\boldsymbol{X}|\{w_{1,}w_{2,}\dots w_{n,}\}\right) = p(\boldsymbol{x}^1)\, p(\boldsymbol{x}^2)\, p(\boldsymbol{x}^3) \dots p(\boldsymbol{x}^P)$$

is maximal is equivalent to maximizing the log-likelihood

$$LL\left(\{w_{1,}w_{2,}\dots w_{n,}\}\right) \quad = \ln(p_{model}) = \sum_k ln\; p(\boldsymbol{x}^k)$$

Note: some people (e.g. David MacKay) use the term 'likelihood' ONLY IF we consider LL($w$) as a function of the parameters $w$.

'likelihood of the model parameters in view of the data'

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## Statistical Classification by Deep Networks

Wulfram Gerstner

EPFL, Lausanne, Switzerland

1. The statistical view: generative model
2. The likelihood of data under a model
3. **Application to artificial neural networks**

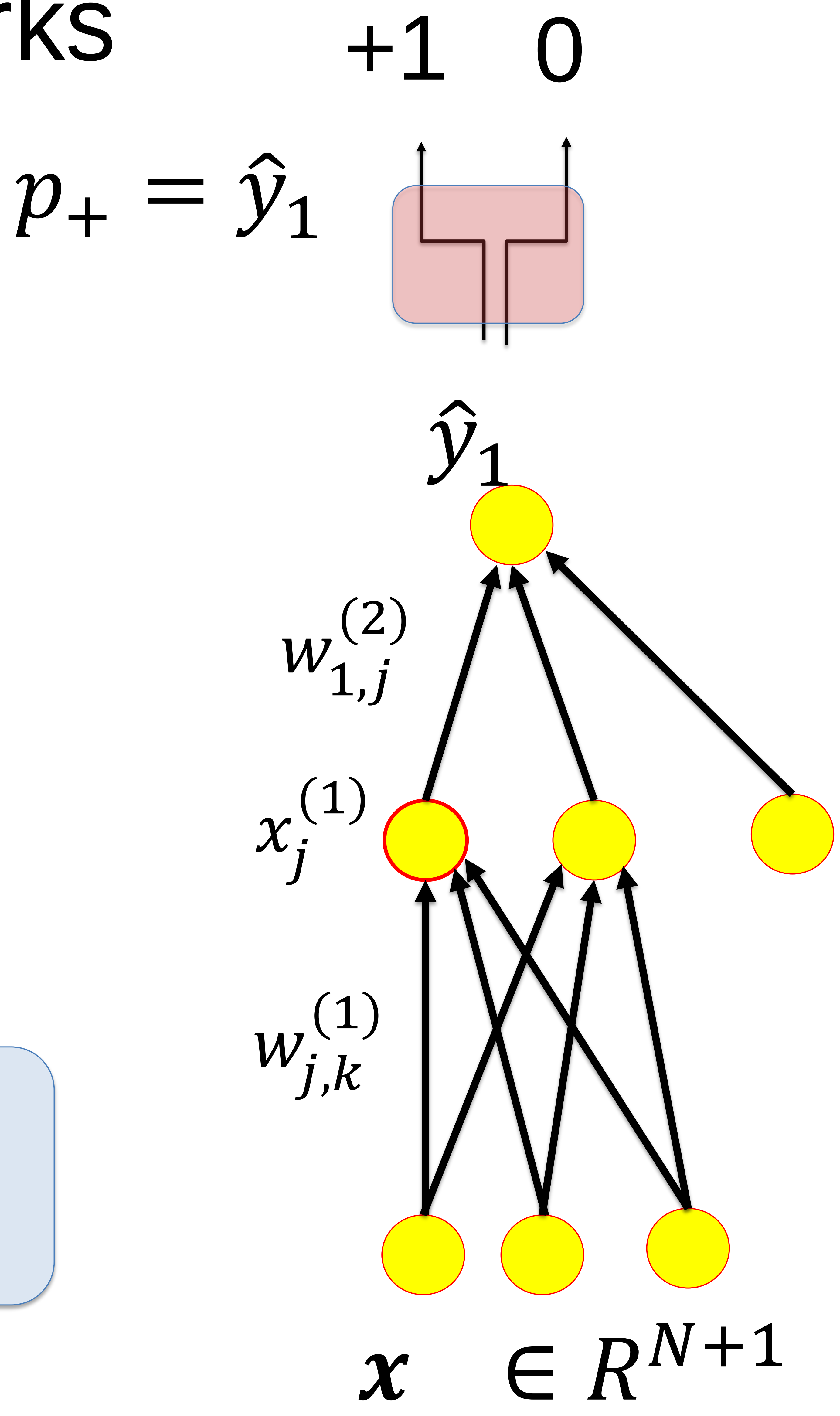
# 3. The likelihood of data under a neural network model

Overall aim:
What is the likelihood that my set of $P$ data points

$$\{ \quad (\boldsymbol{x}^{\mu}, t^{\mu}) \quad , \qquad 1 \leq \mu \leq P \quad \};$$

**could have been generated** by my model?

# 3. Maximum Likelihood for neural networks



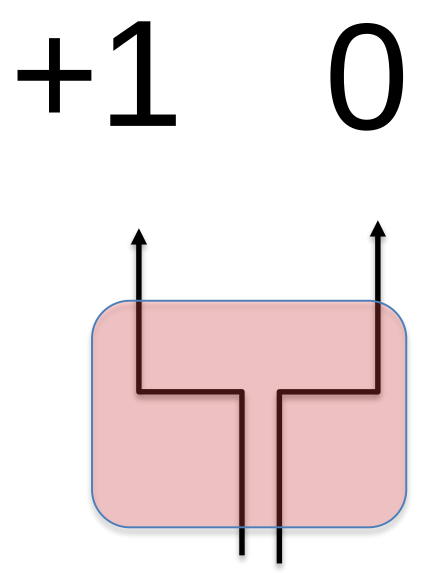

*Blackboard 3:*
Likelihood of $P$ input-output pairs

*Blackboard 3:*

Likelihood of $P$ input-output pairs

# 3. Maximum Likelihood for neural networks

$p_+ = \hat{y}_1$

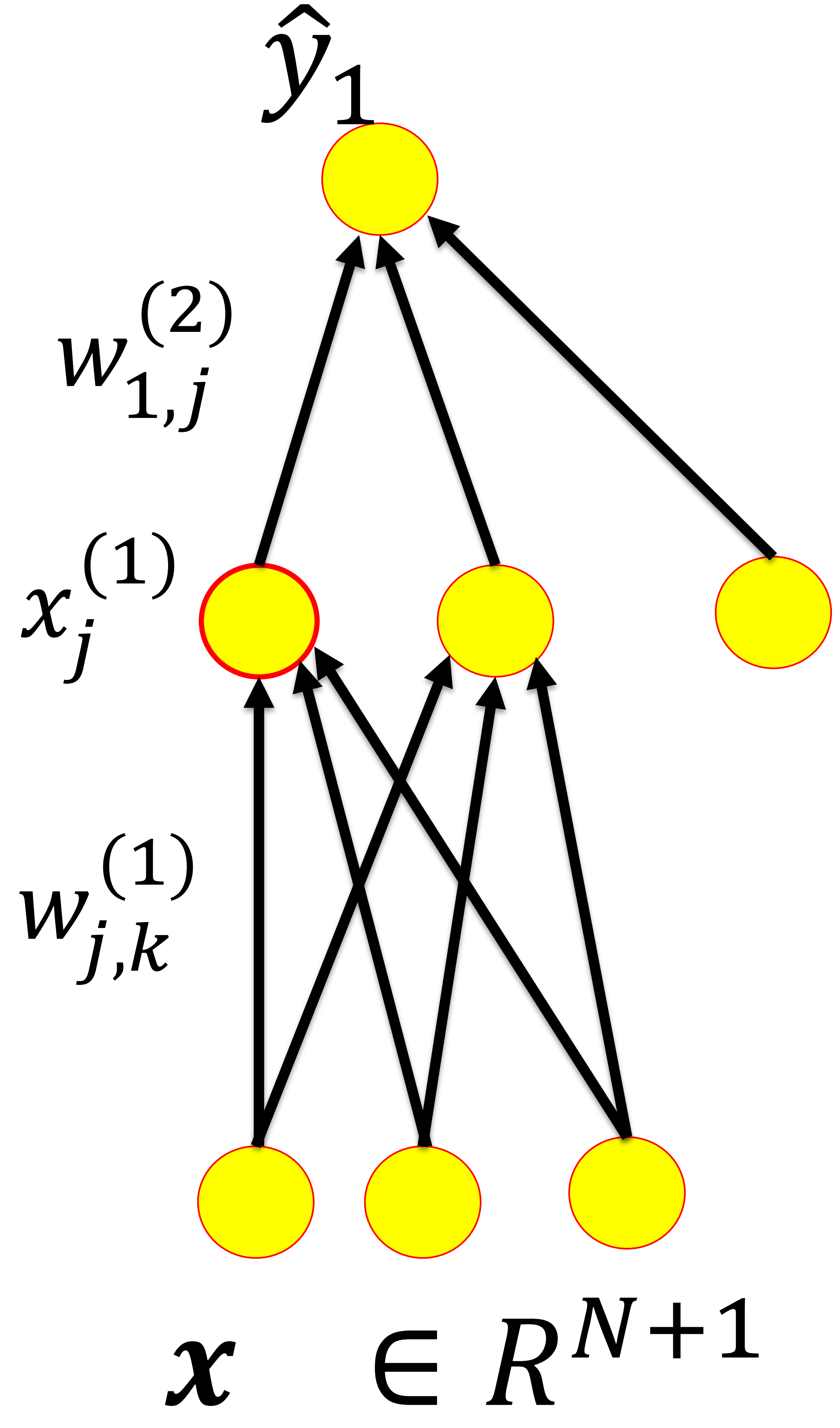



Minimize the negative log-likelihood

$$E(w) = -LL = -\ln(p_{model})$$

parameters= all weights, all layers

$$E(w) = -\sum_\mu [t^\mu \, ln \, \hat{y}^\mu + (1 - t^\mu)\ln(1 - \hat{y}^\mu)]$$



# 3. Cross-entropy error function for neural networks

Suppose we minimize the cross-entropy error function

$$E(w) = -\sum_\mu [t^\mu \, ln \, \hat{y}^\mu + (1 - t^\mu) \ln(1 - \hat{y}^\mu)]$$

Can we be sure that the output $\hat{y}^\mu$ will represent the probability?

Intuitive answer: **No, because**

A We will need enough data for training

(not just 10 data points for a complex task)

B We need a sufficiently flexible network

(not a simple perceptron for XOR task)

# 3. Output = probability ?

Suppose we minimize the cross-entropy error function

$$E(w) = -\sum_{\mu}[t^{\mu}\, ln\, \hat{y}^{\mu} + (1 - t^{\mu})\ln(1 - \hat{y}^{\mu})]$$

Assume

A We have enough data for training

B We have a sufficiently flexible network

*Blackboard 4:*

From Cross-entropy to output probabilities

*Blackboard 4:*

From Cross-entropy to output probabilities

QUIZ: **Maximum likelihood solution** means

[ ] find the unique set of parameters that generated the data

[ ] find the unique set of parameters that best explains the data

[ ] find the best set of parameters such that your model could have generated the data

Miminization of the **cross-entropy error** function for single class output

[ ] is consistent with the idea that the output $\hat{y}_1$ of your network can be interpreted as $\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x})$

[ ] guarantees that the output $\hat{y}_1$ of your network can be interpreted as $\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x})$

# Artificial Neural Networks: Lecture 3

## Statistical Classification by Deep Networks

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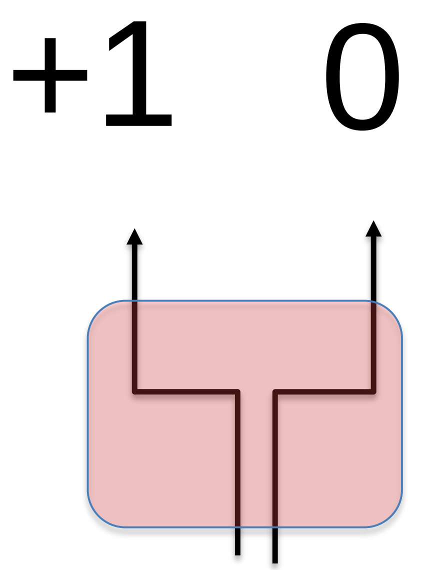
1. The statistical view: generative model
2. The likelihood of data under a model
3. Application to artificial neural networks
4. **Sigmoidal as a natural output function**

# 4. Why sigmoidal output ? – single class

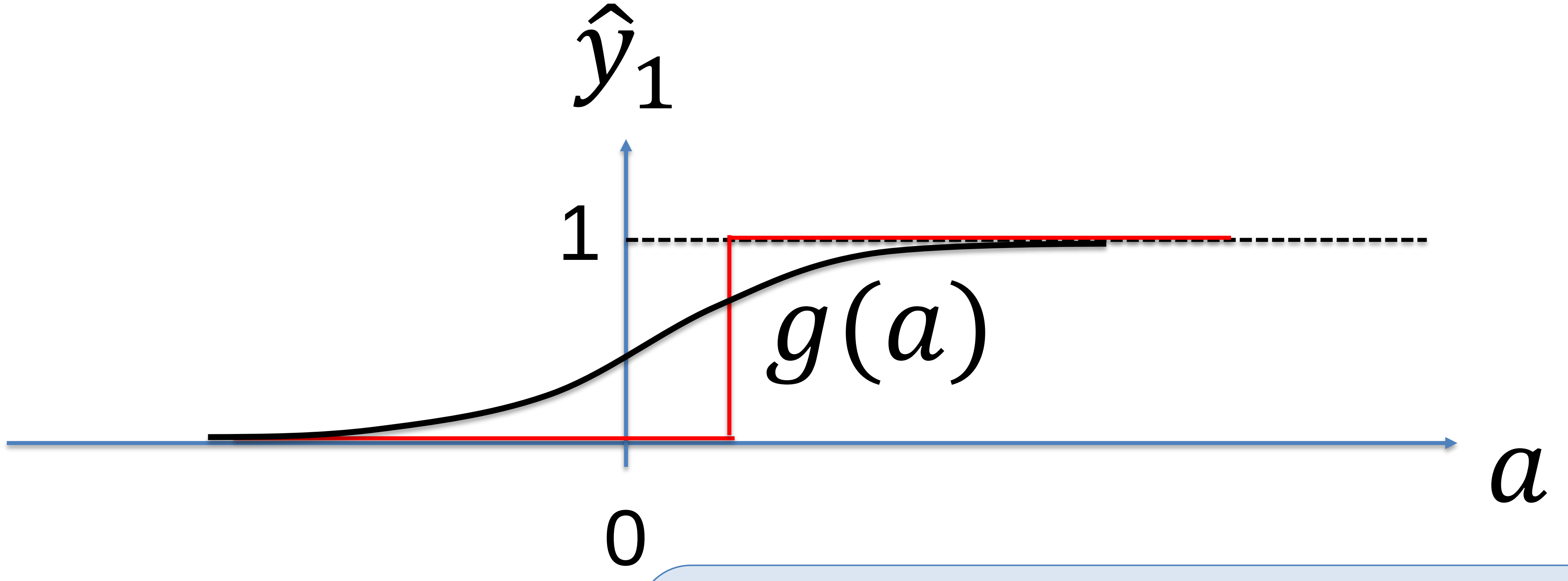
$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

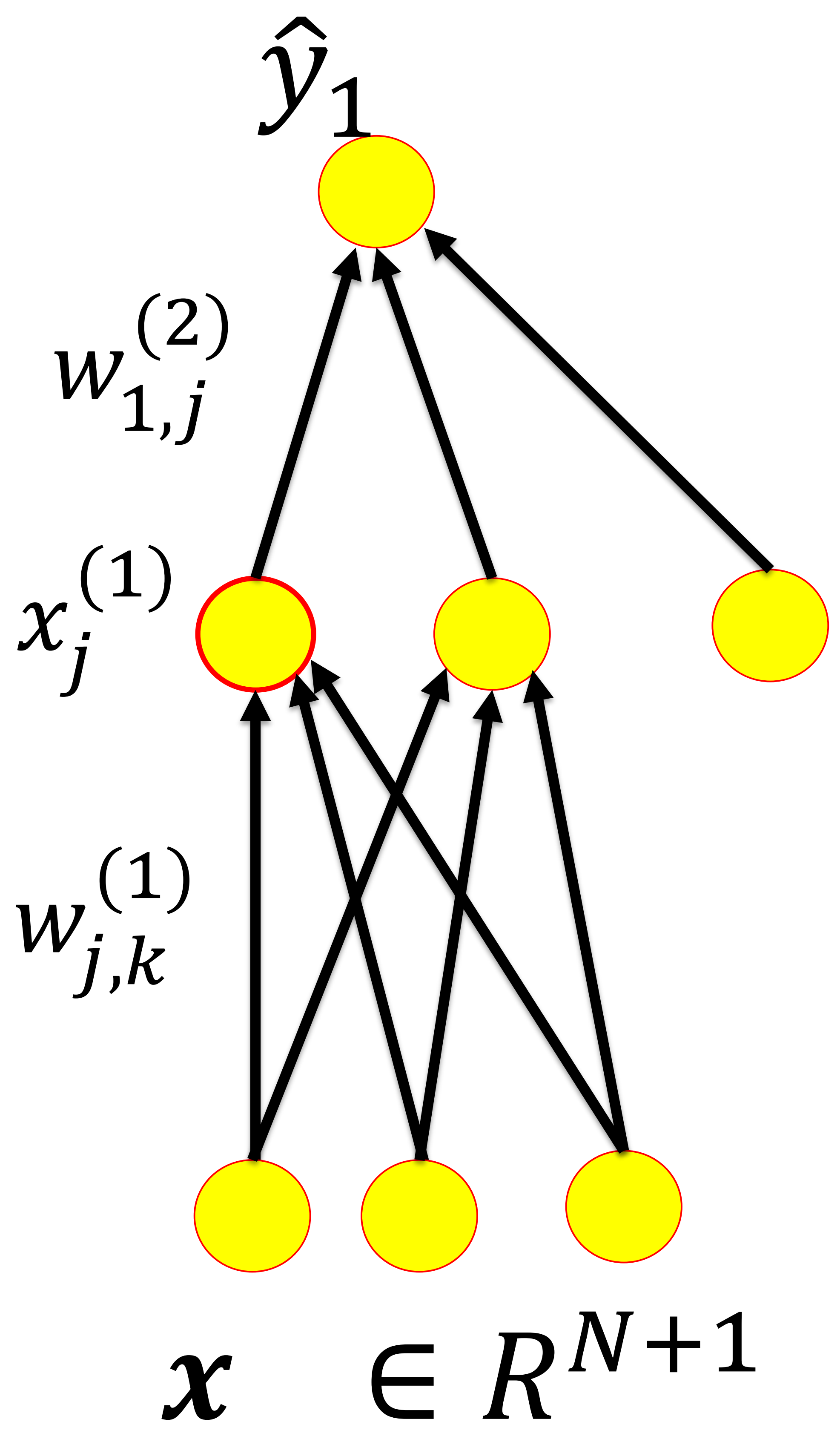
$p_+ = \hat{y}_1$  $p_- = 1 - \hat{y}_1$



**Observations (single-class):**

- Probability must be between 0 and 1
- Inutitively: smooth is better




*Blackboard 5:*
derive optimal sigmoidal

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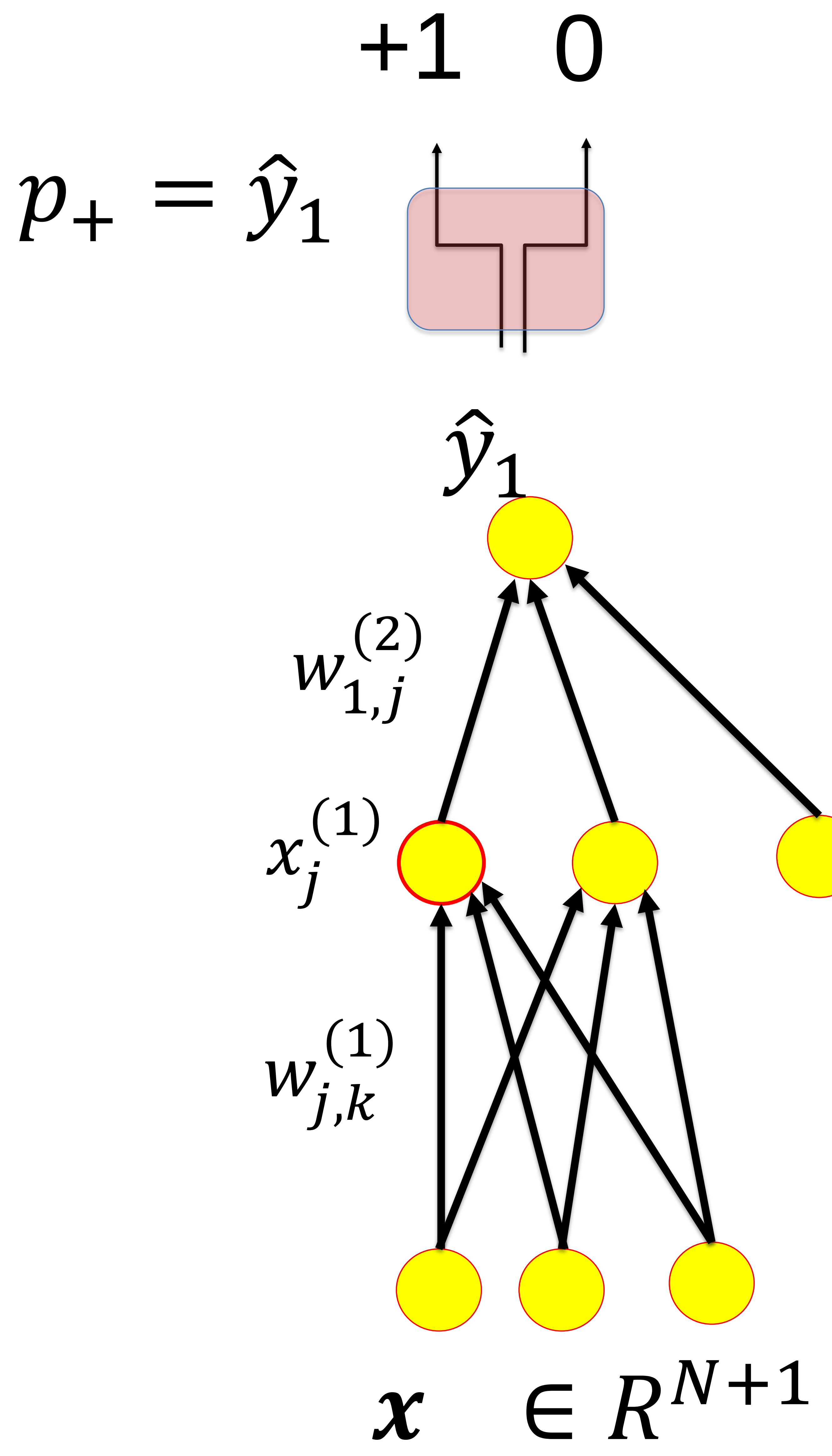
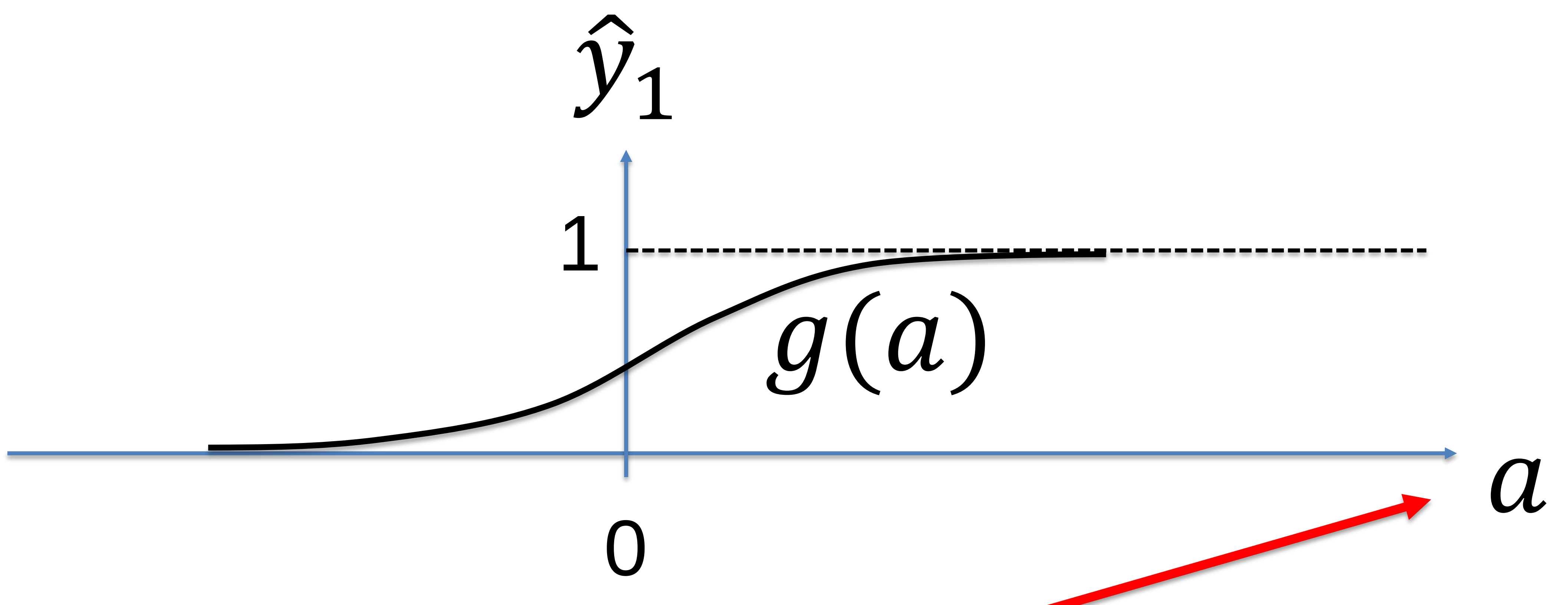
derive optimal sigmoidal



# 4. Why sigmoidal output ? – single class

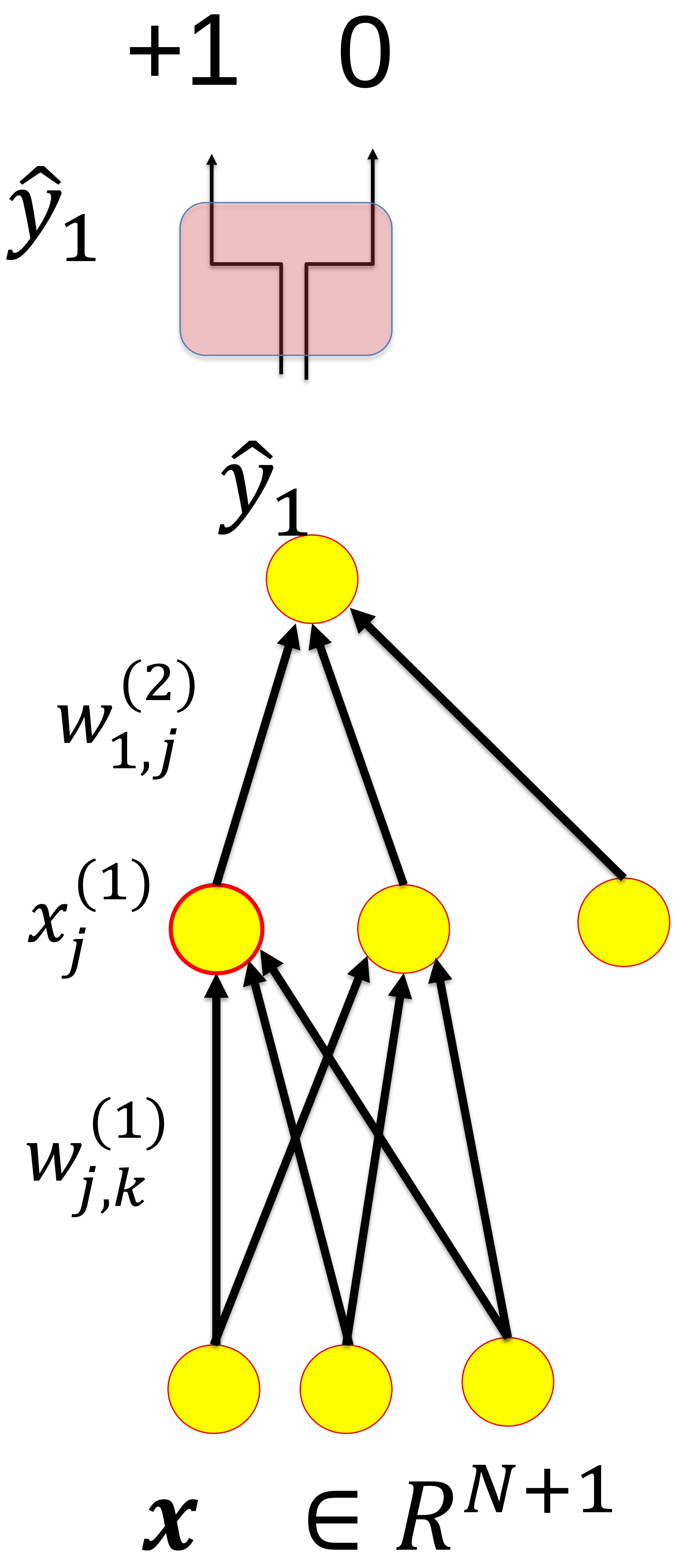
$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

$$\hat{y}_1 = g(a) = \frac{1}{1+e^{-a}}$$




total input $a$ into output neuron can be interpreted as log-prob. ratio

$p_+ = \hat{y}_1$



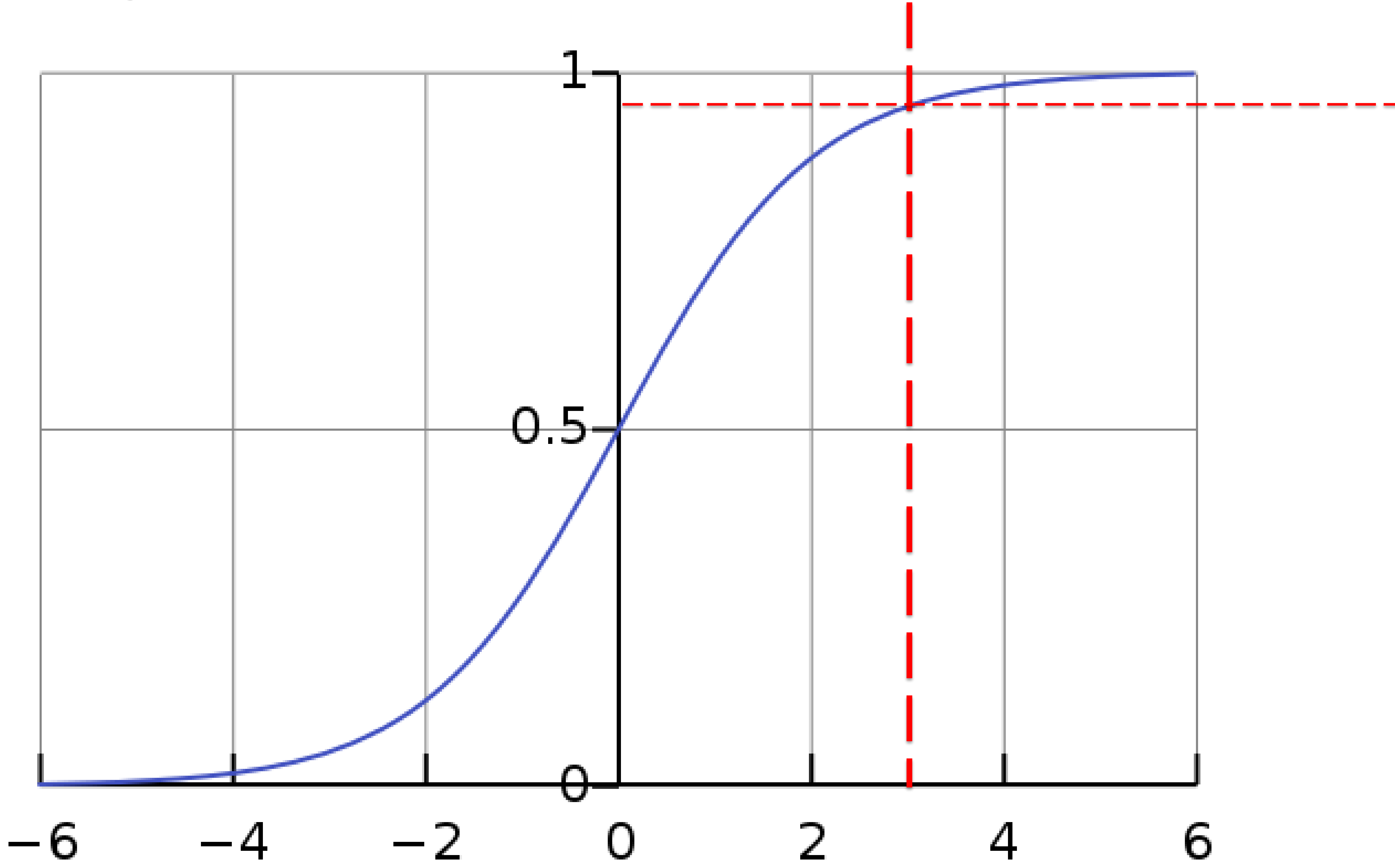
# 4. sigmoidal output **= logistic function**

$$g(a) = \frac{1}{1 + e^{-a}}$$

Rule of thumb:

for $a = 3$: $g(3) = 0.95$

for $a = -3$: $g(-3) = 0.05$




https://en.wikipedia.org/wiki/Logistic_function

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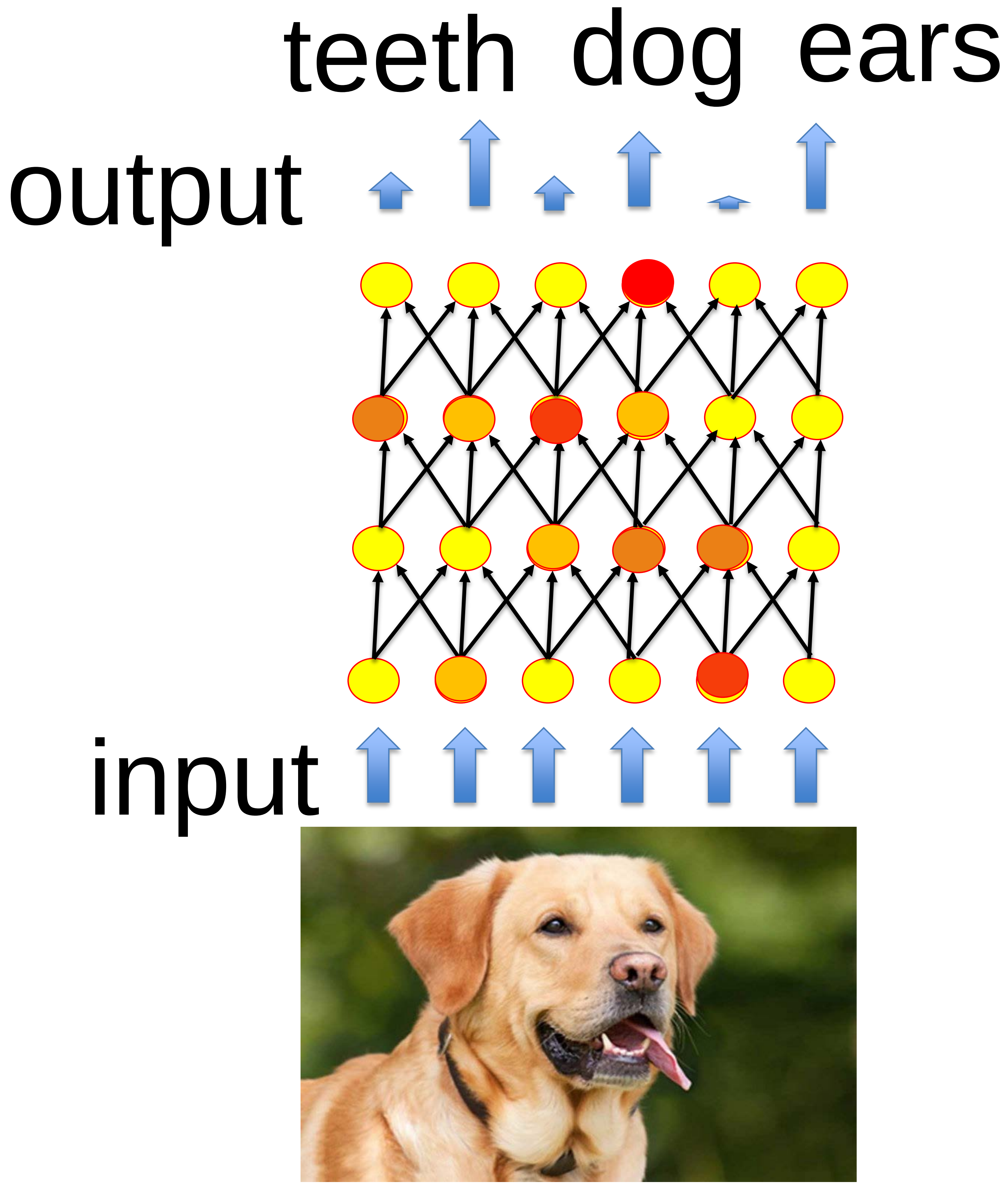
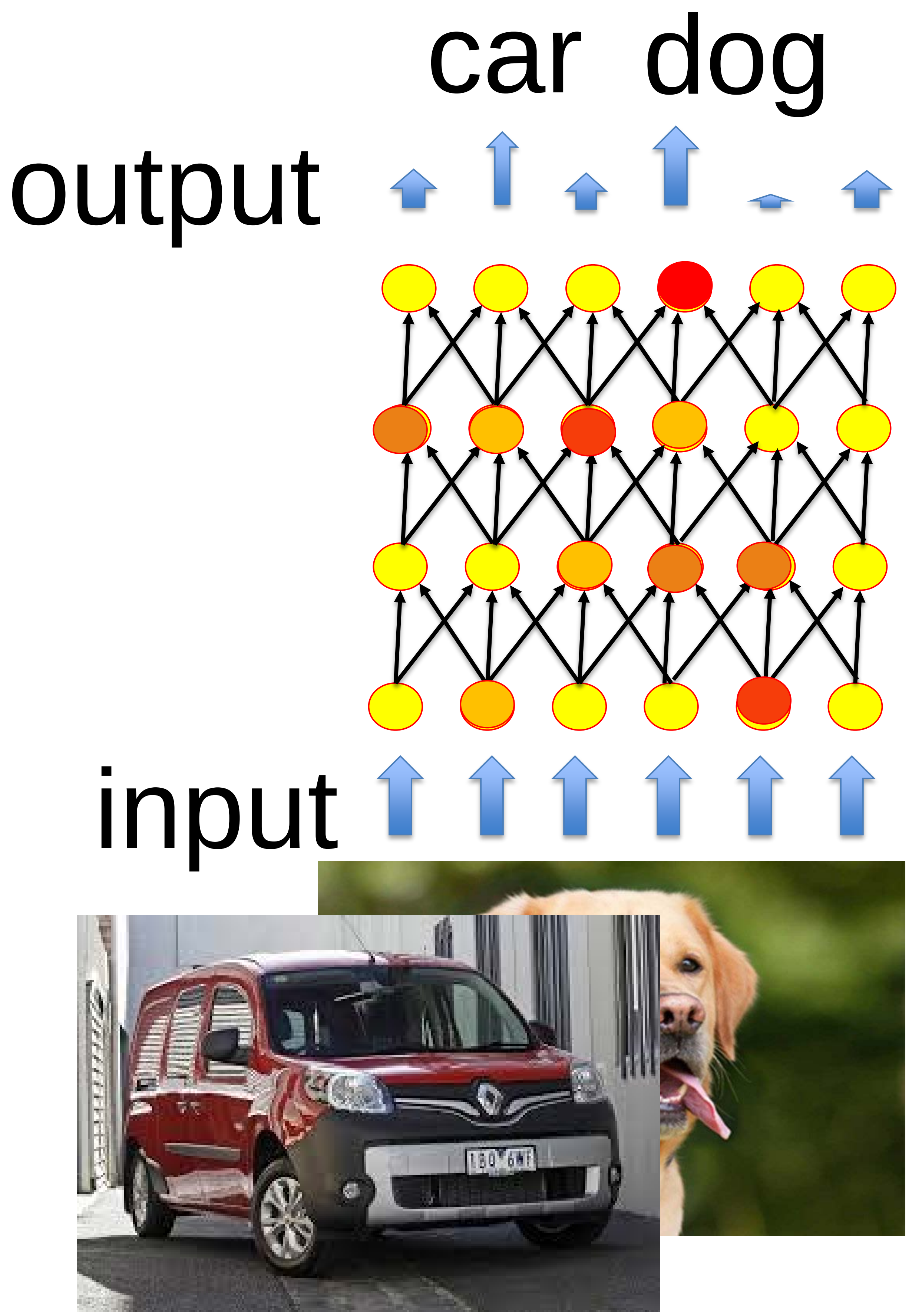
3. Application to artificial neural networks
4. Sigmoidal as a natural output function
5. **Multi-class problems**

# 5. Multiple Classes

**multiple attributes**

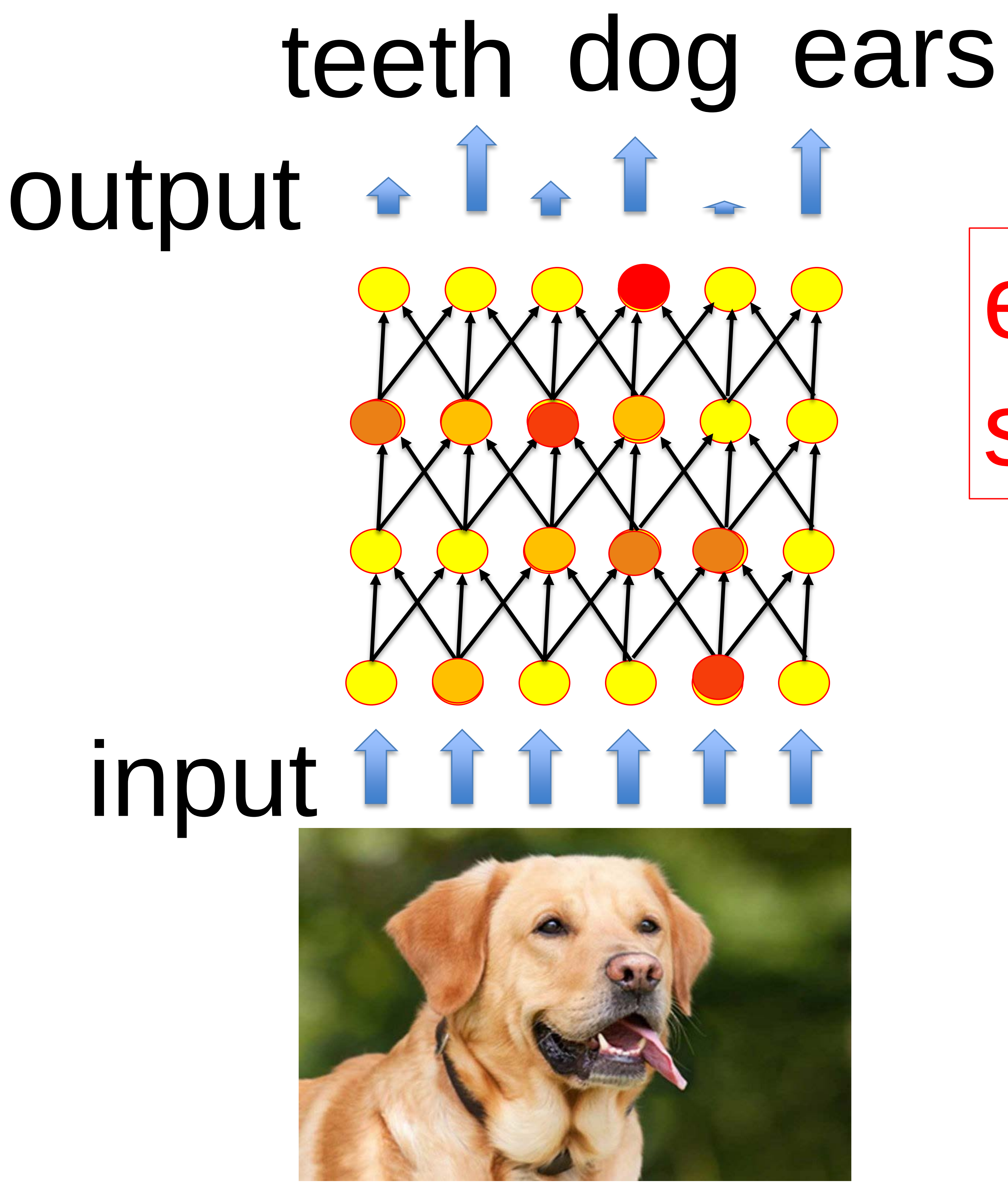



**mutually exclusive classes**

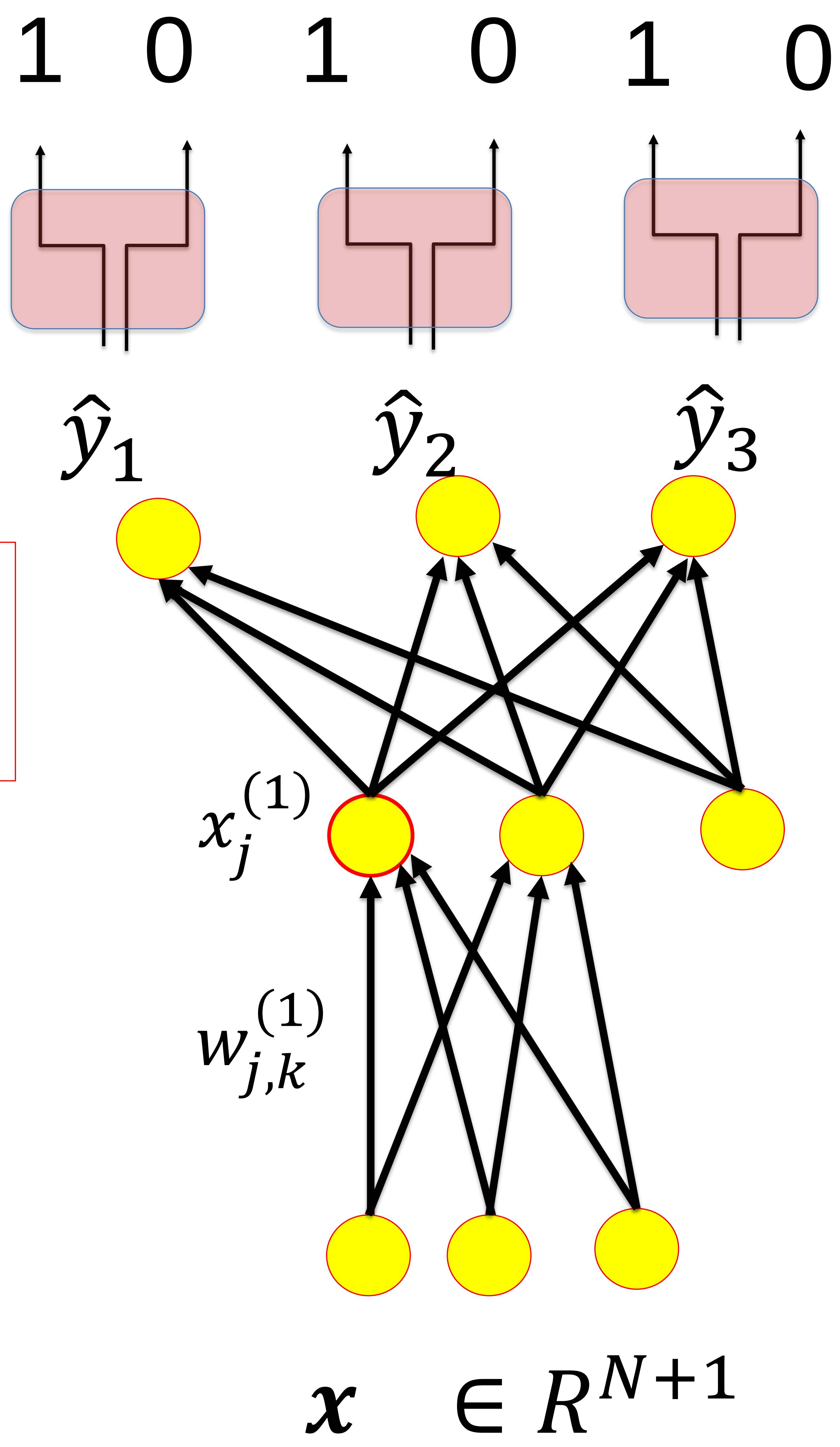


# 5. Multiple Classes: Multiple attributes

Multiple attributes:



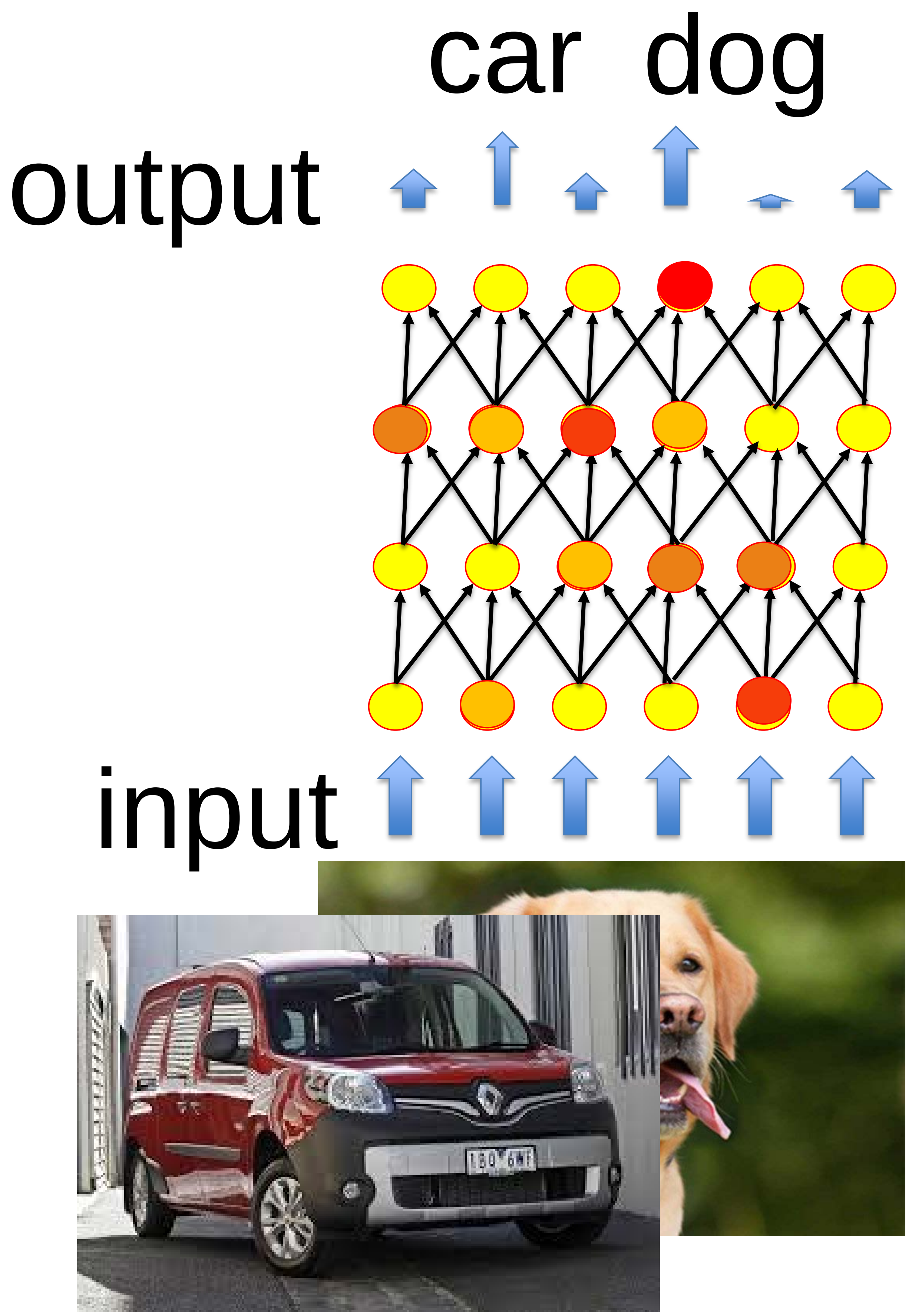

equivalent to several single-class decisions



# 5. Multiple Classes: Mutuall exclusive classes

mutually exclusive classes

either car or dog:
only one can be true
→
outputs interact

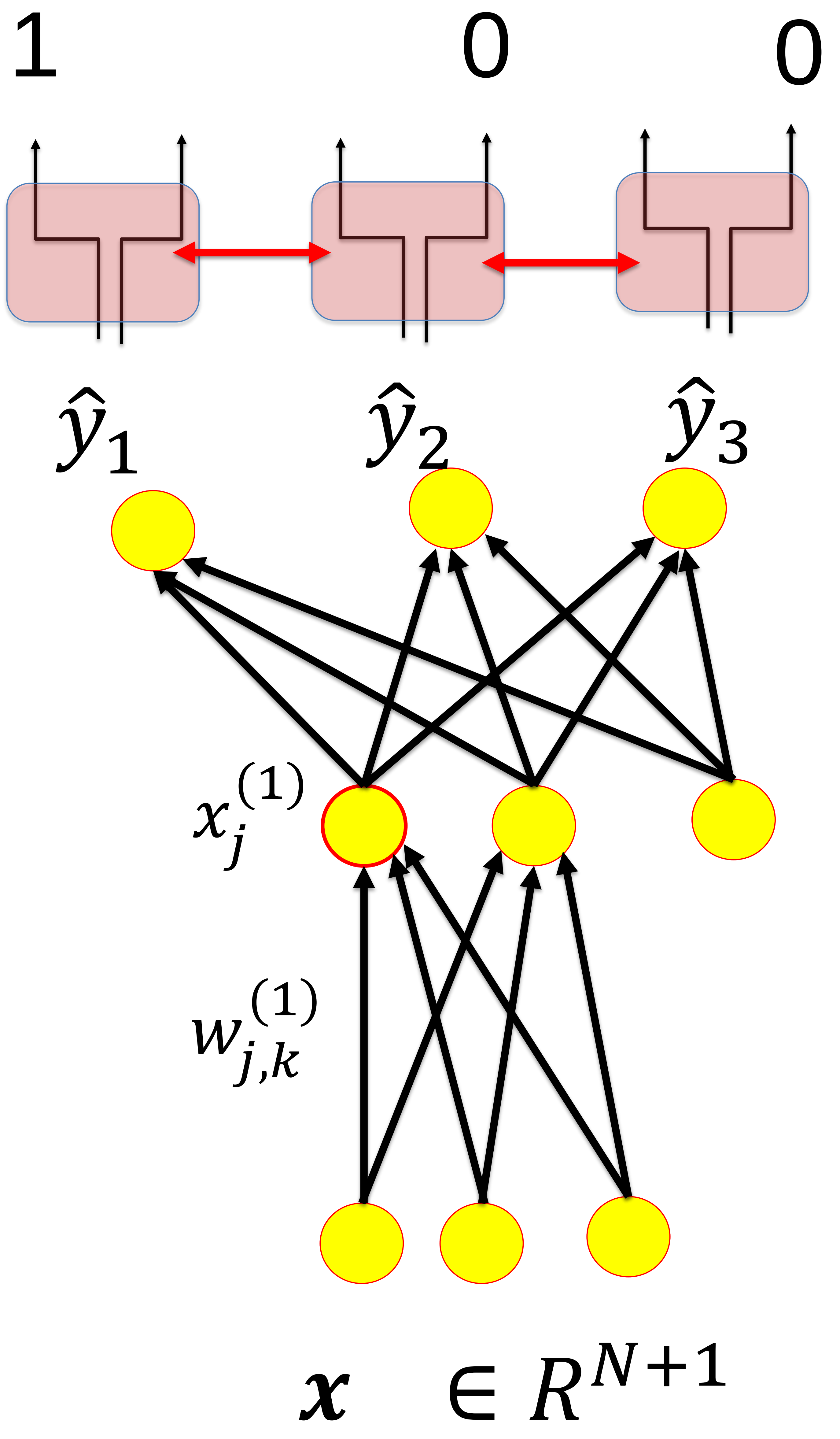


# 5. Exclusive Multiple Classes

$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

1-hot-coding:

$$\hat{t}_k^\mu = 1 \rightarrow \quad \hat{t}_j^\mu = 0 \text{ for } j \neq k$$



# 5. Exclusive Multiple Classes

$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

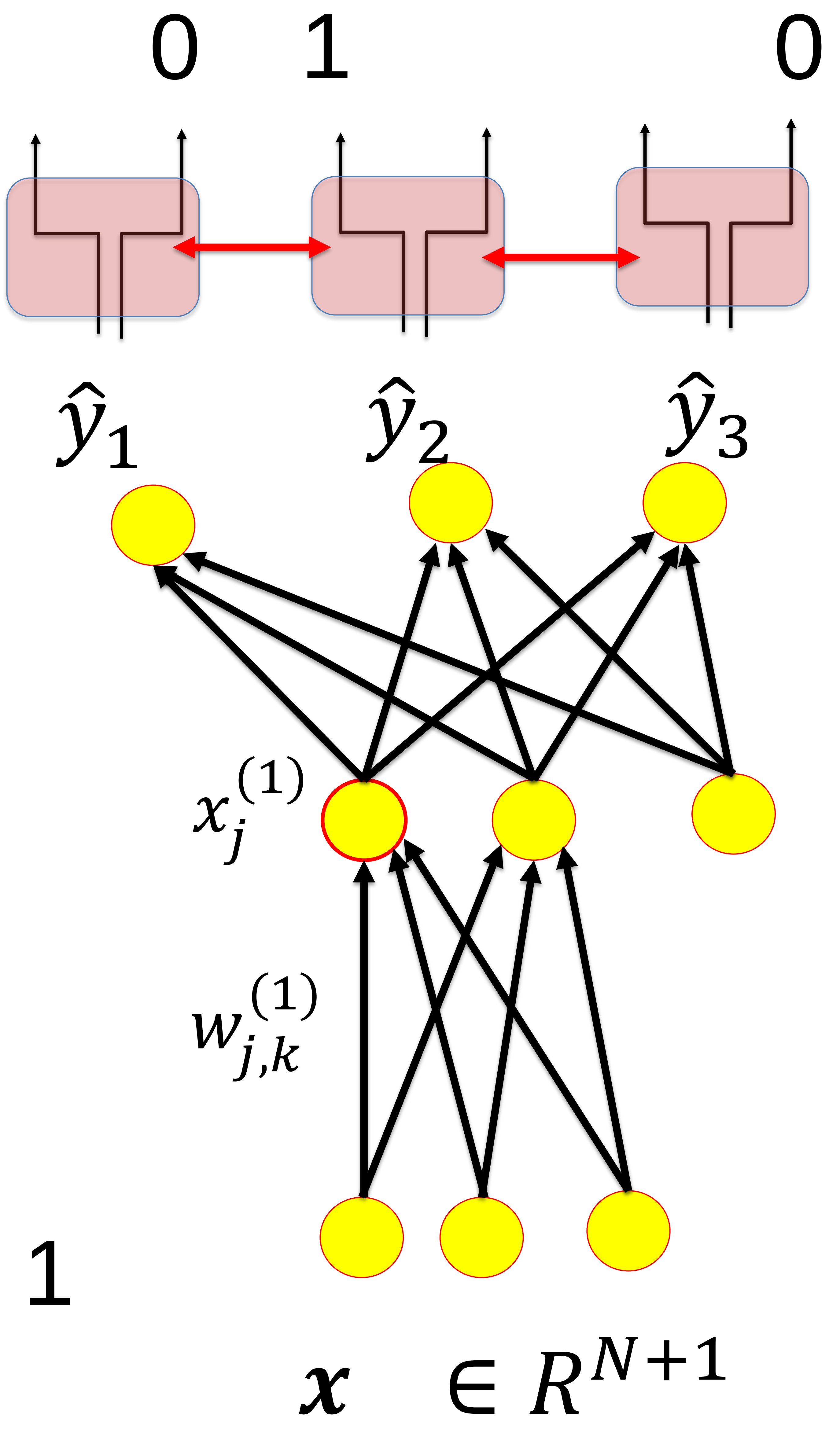
1-hot-coding:

$$\hat{t}_k^{\mu} = 1 \rightarrow \quad \hat{t}_j^{\mu} = 0 \text{ for } j \neq k$$

Outputs are NOT independent:

$$\sum_{k=1}^{K} t_k^{\mu} = 1$$ exactly one output is 1

$$\sum_{k=1}^{K} \hat{y}_1^{\mu} = 1$$ Output probabilities sum to 1

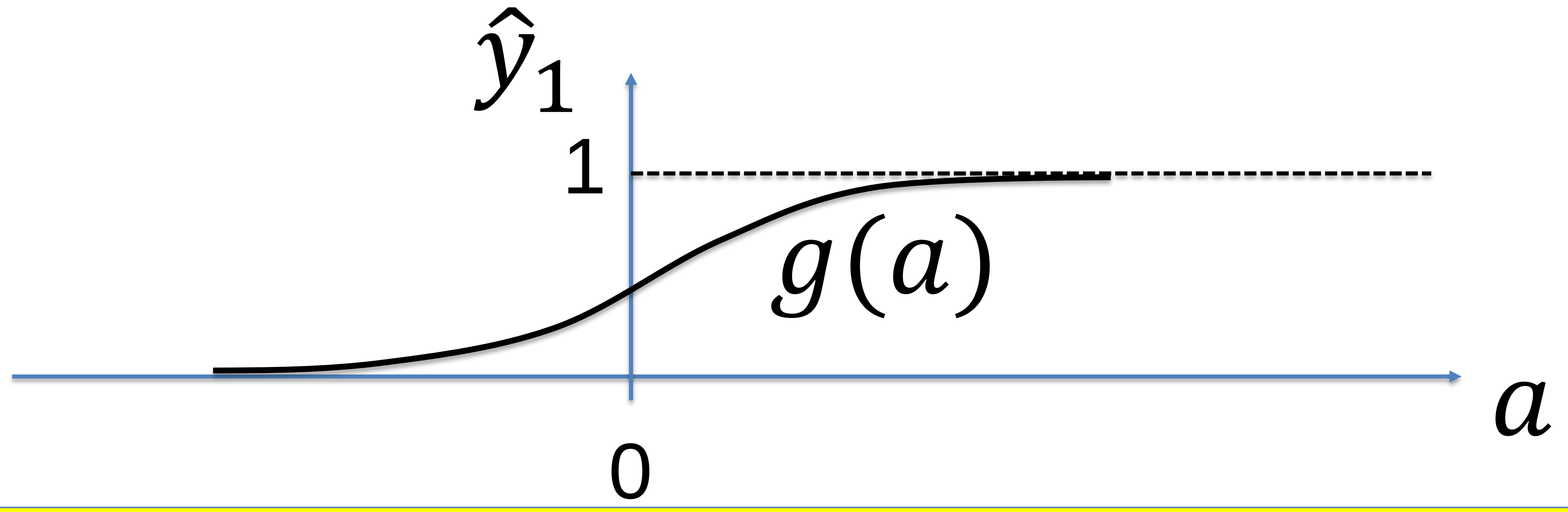


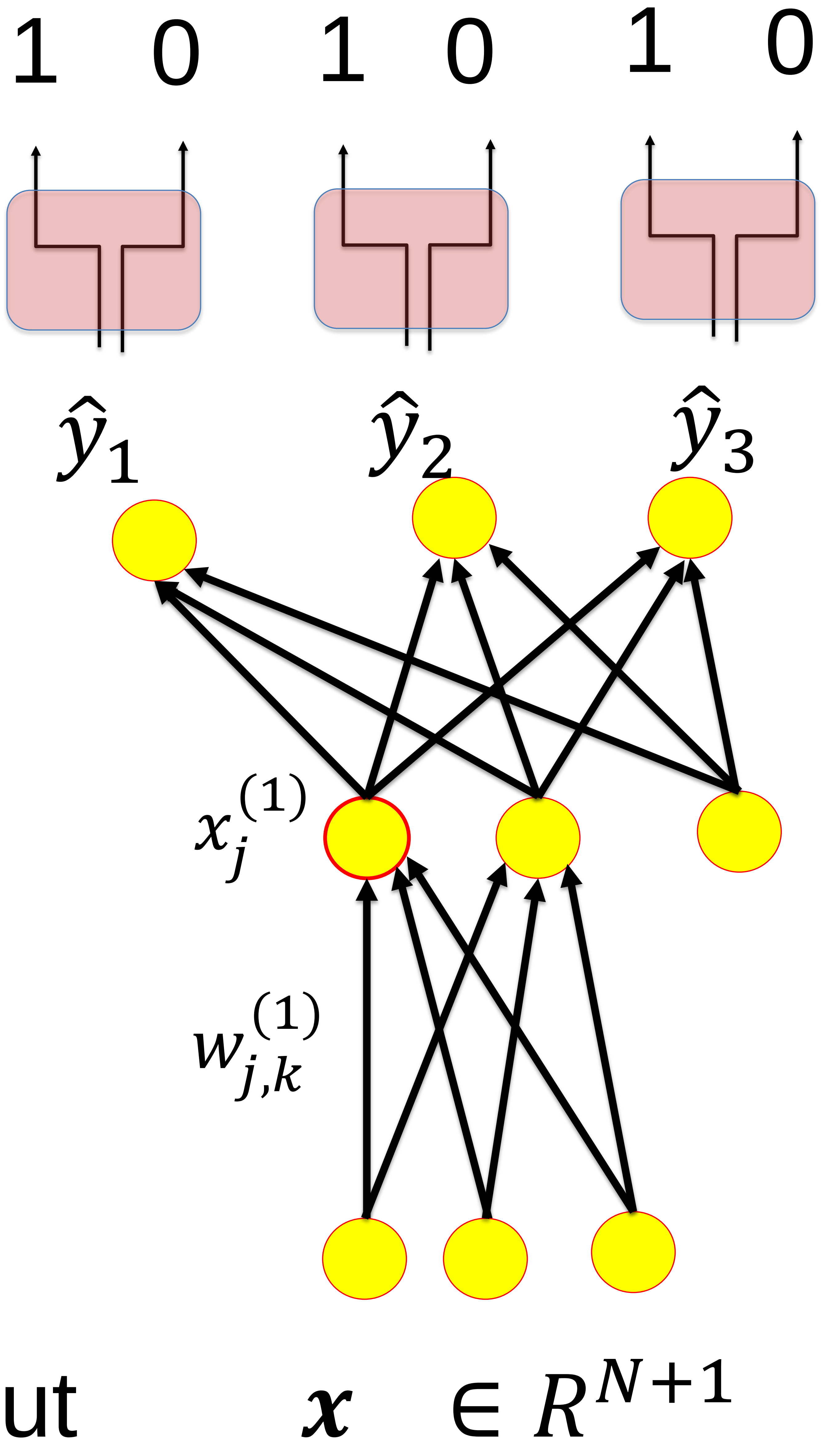
# 5. Why sigmoidal output ?

$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

**Observations (multiple-classes):**

- Probabilities must sum to one!



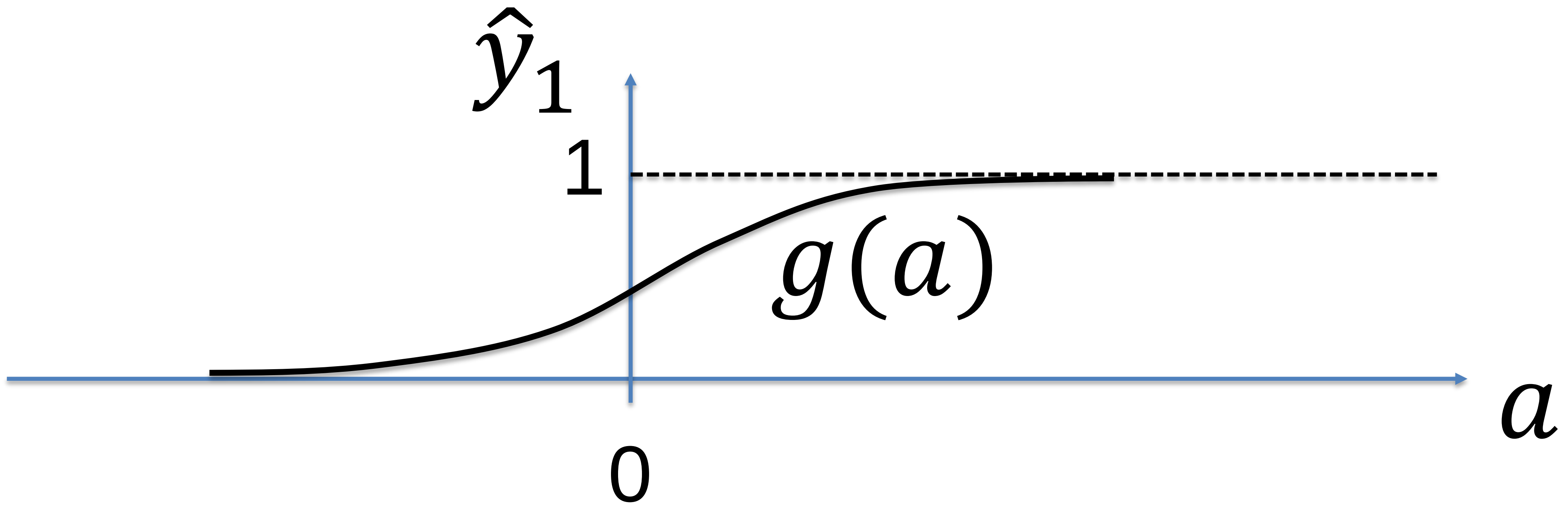



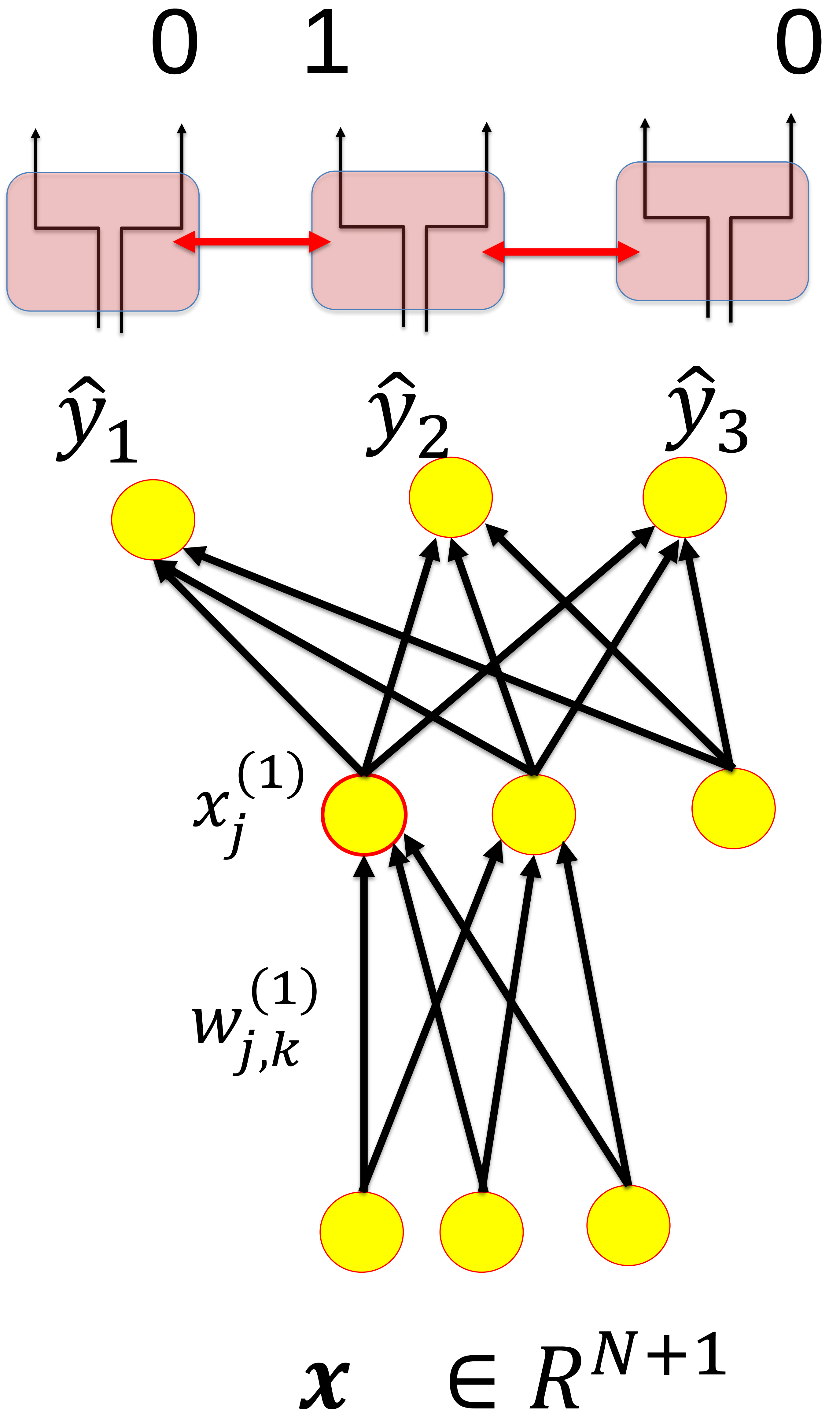

*Exercise this week!*
derive softmax as optimal multi-class output

# 5. Softmax output

$$\hat{y}_k = \mathrm{P}(C_k|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_k = 1|\boldsymbol{x})$$

$$\hat{y}_k = \mathrm{P}(C_k|\boldsymbol{x}) = \frac{\boldsymbol{exp}(a_k)}{\sum_j \boldsymbol{exp}(a_j)}$$



# 5. Exclusive Multiple Classes

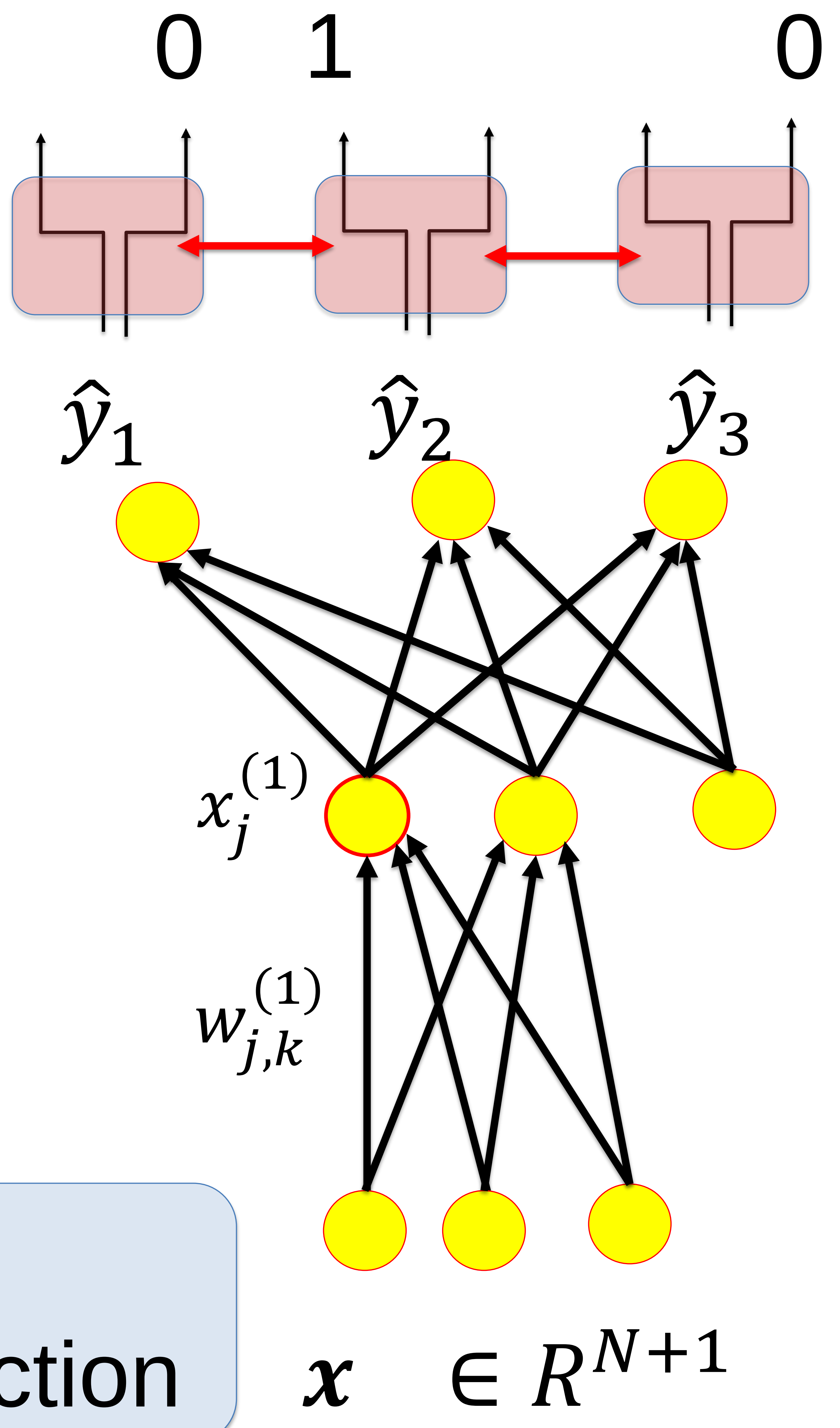
$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

1-hot-coding:

$$\hat{t}_k^{\mu} = 1 \rightarrow \hat{t}_j^{\mu} = 0 \text{ for } j \neq k$$

Outputs are NOT independent:

$$\sum_{k=1}^{K} t_k^{\mu} = 1$$ exactly one output is 1




*Blackboard 6:*
probility of target labels and likelihood function

*Blackboard 6:*

Probability of target labels: mutually exclusive classes

# 5. Cross entropy error for neural networks: Multiclass

We have a total of $K$ classes (mutually exclusive: either dog or car)

Minimize* the **cross-entropy**

$$E(w) = -\sum_{k=1}^{K} \sum_{\mu} [t_k^\mu \, ln \, \hat{y}_k^\mu]$$

parameters= all weights, all layers

*Minimization under the constraint:
$\sum_{k=1}^{K} \hat{y}_k^\mu = 1$

Compare: **KL divergence between outputs and targets**

$$\text{KL}(w) = -\{\sum_{k=1}^{K} \sum_\mu [t_k^\mu ln \, \hat{y}_k^\mu] - \sum_\mu [t_k^\mu ln \, t_k^\mu]\}$$

$$\text{KL}(w) = E(w) + constant$$

# Artificial Neural Networks: Lecture 3

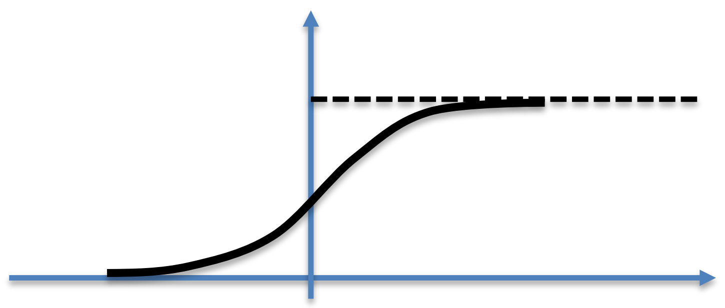
## Statistical Classification by Deep Networks

Wulfram Gerstner

EPFL, Lausanne, Switzerland

1. The statistical view: generative model
2. The likelihood of data under a model
3. Application to artificial neural networks
4. Multi-class problems
5. Sigmoidal as a natural output function
6. **Rectified linear for hidden units**

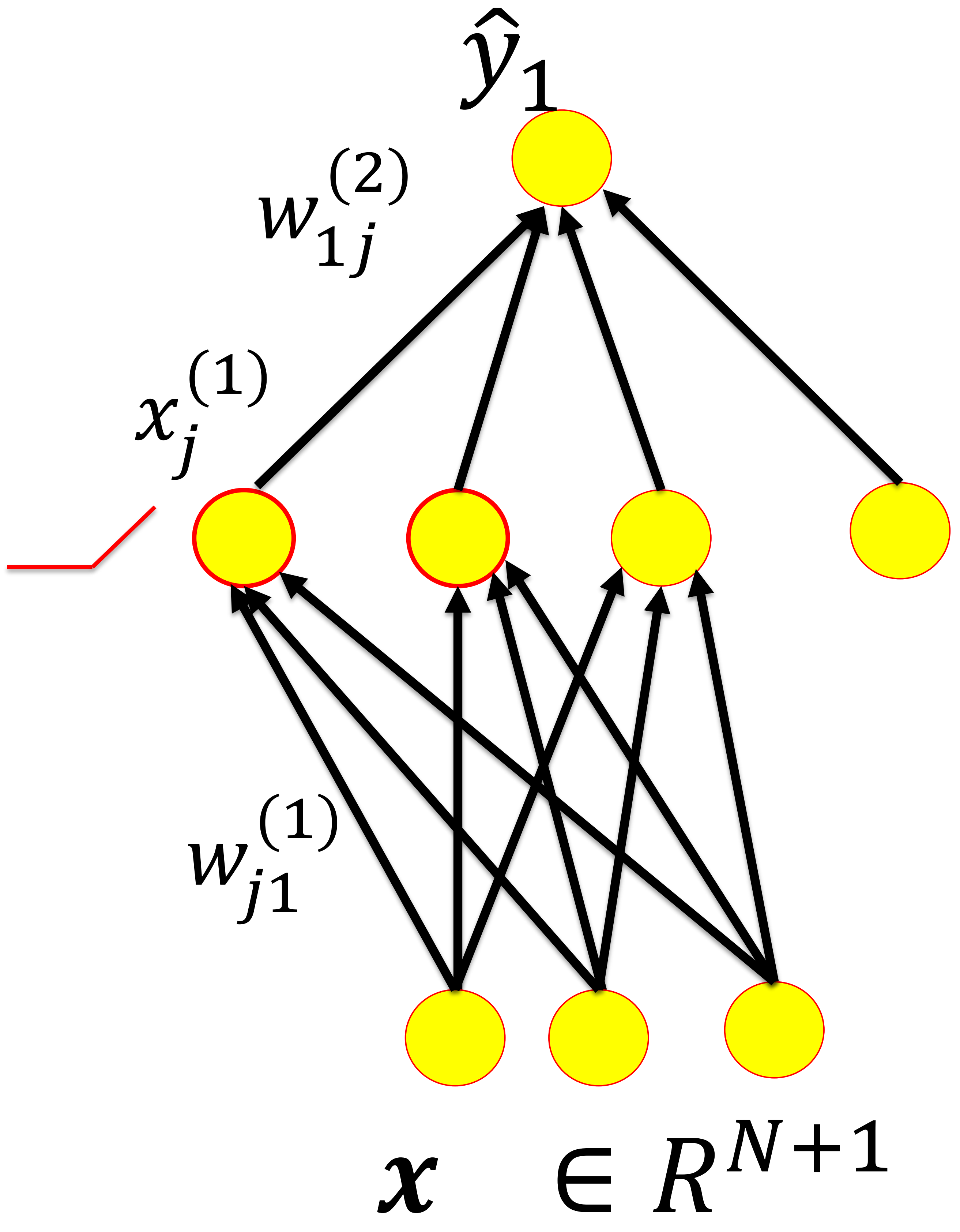
# 6. Modern Neural Networks



**output layer**

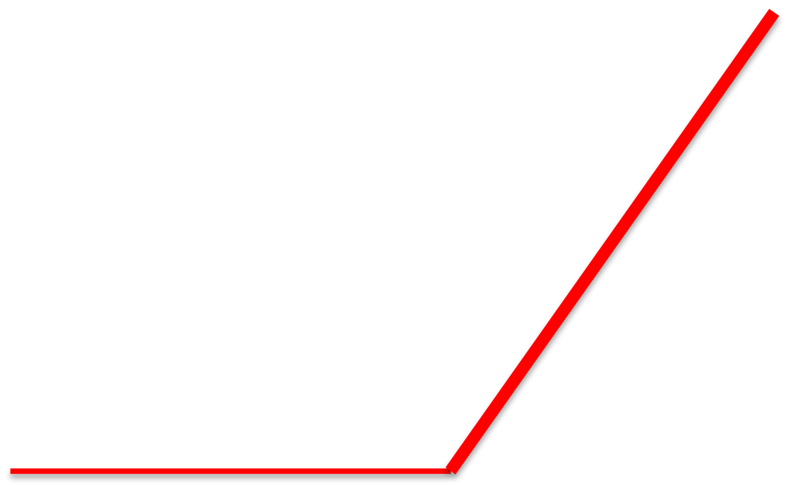
use sigmoidal unit (single-class)

or softmax (exclusive mutlit-class)




**hidden layer**

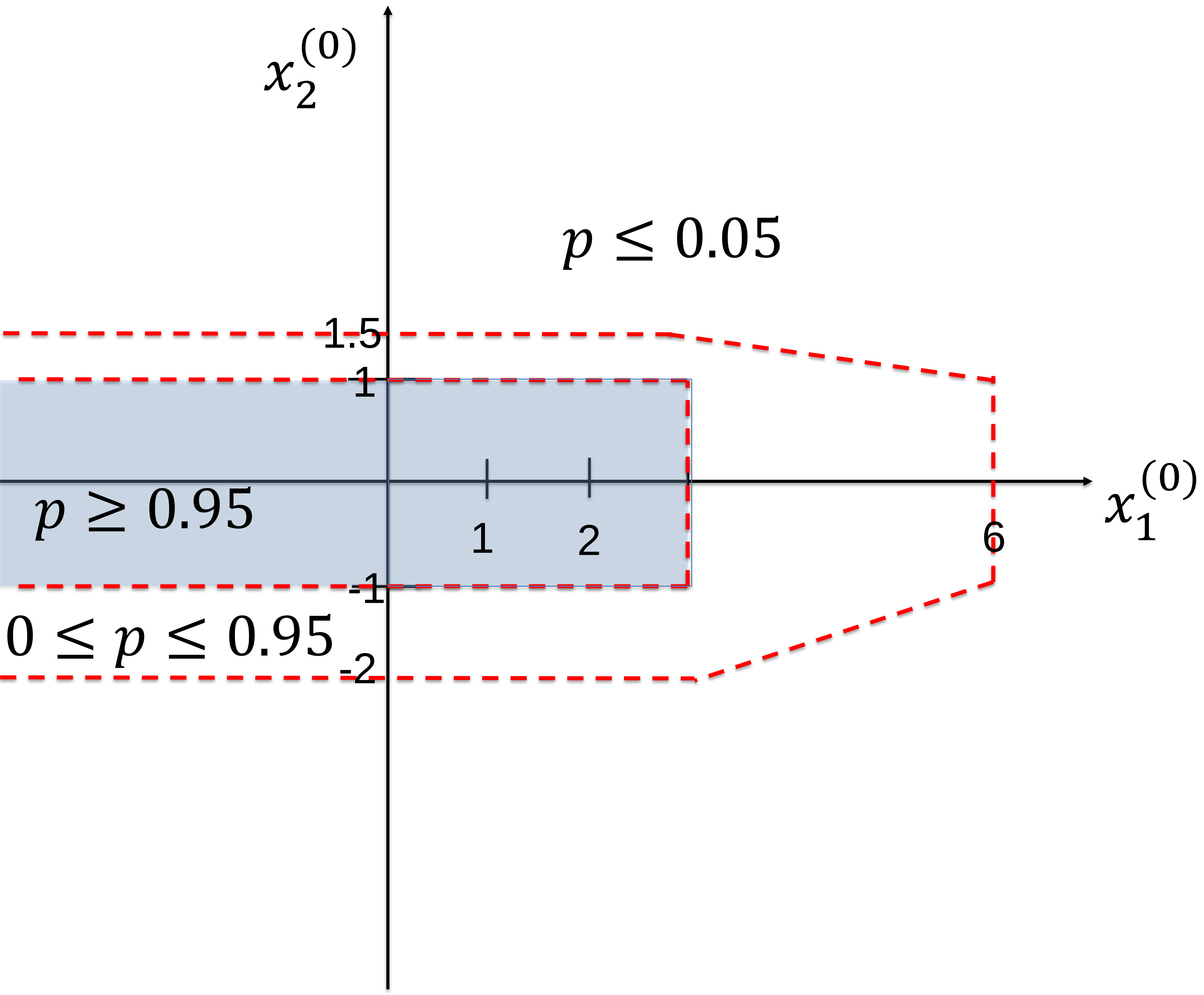
use rectified linear unit in $N+1$ dim.

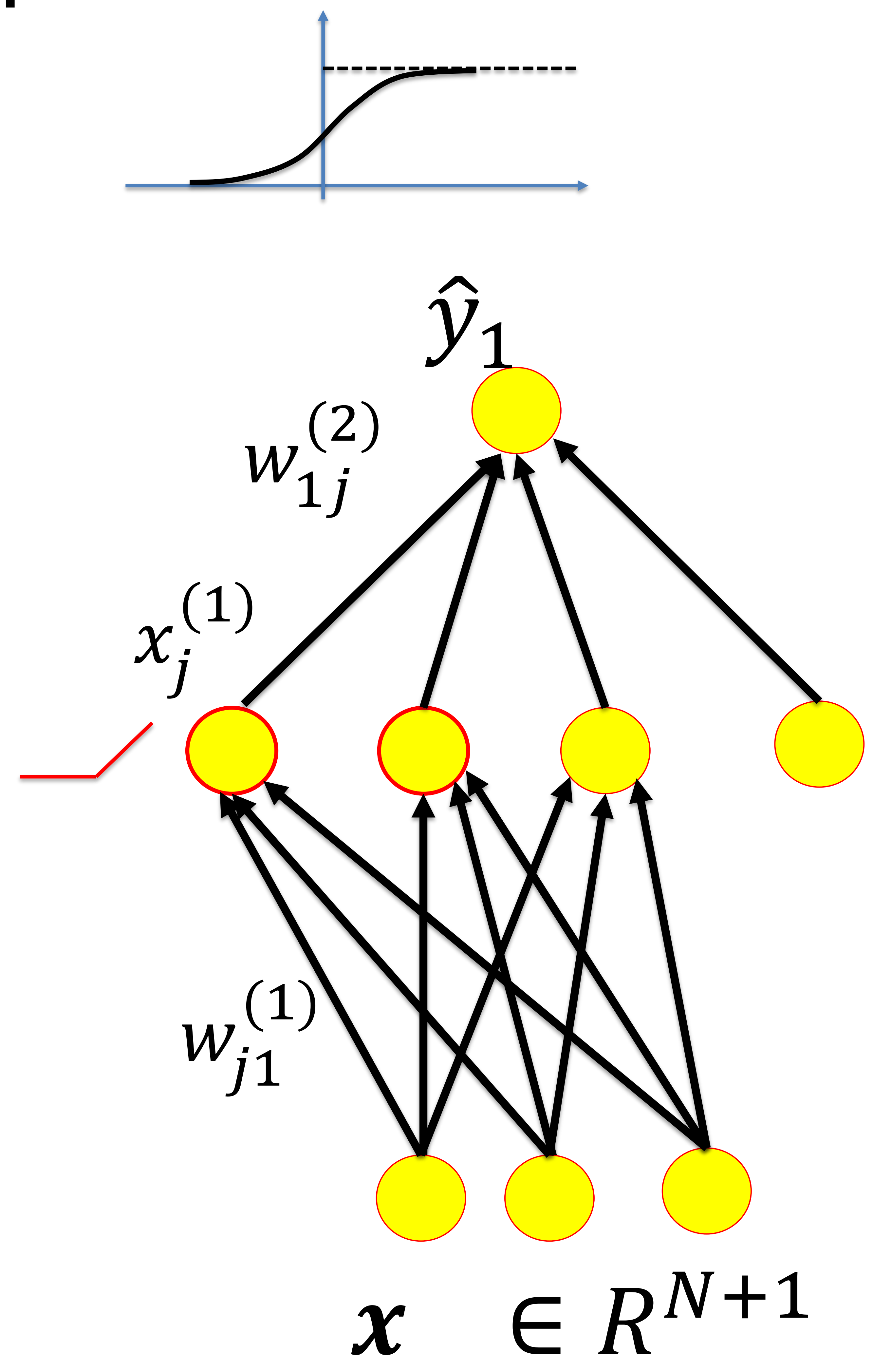


$f(x)=x$ for $x>0$

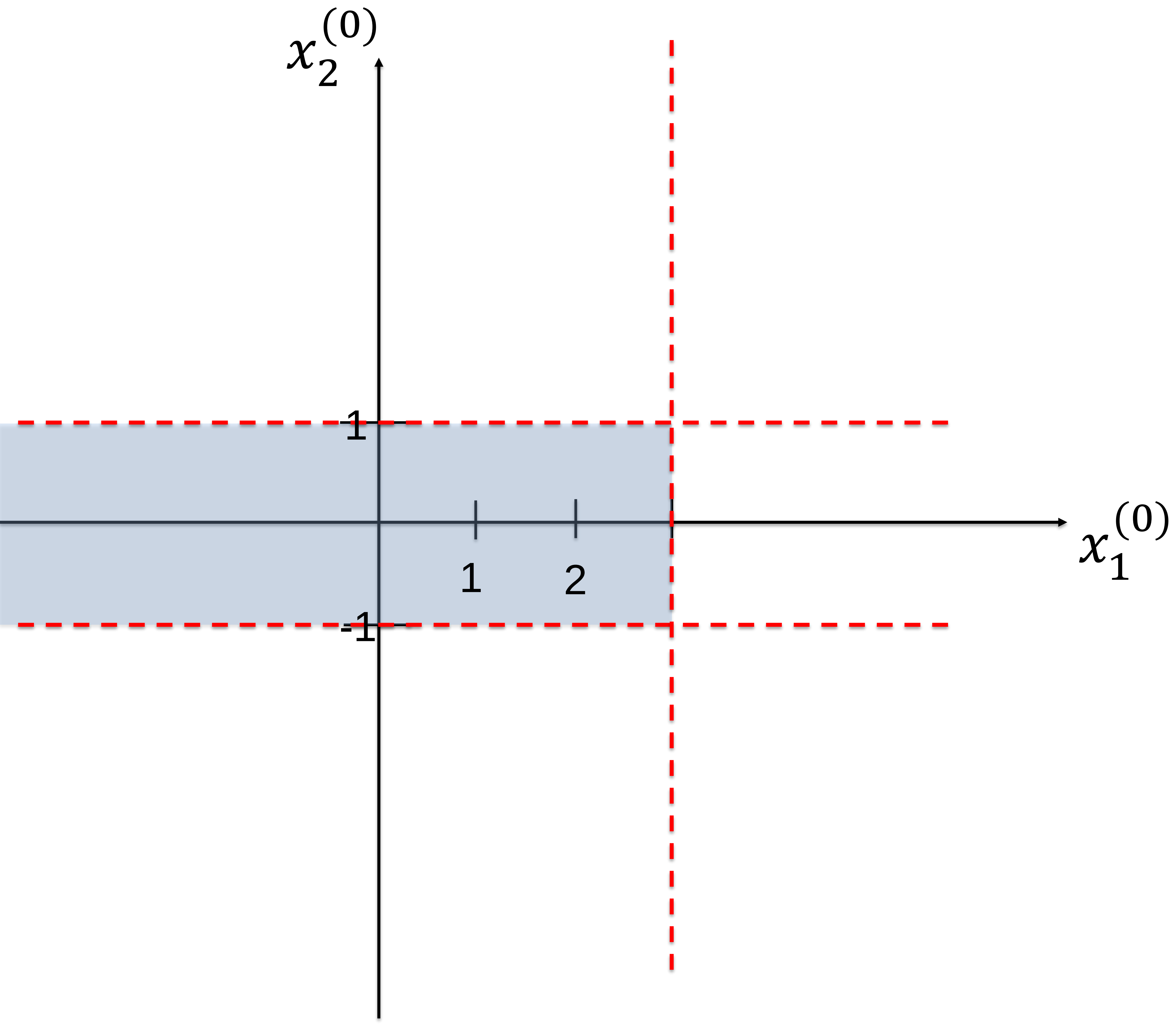
$f(x)=0$ for $x<0$ or $x=0$

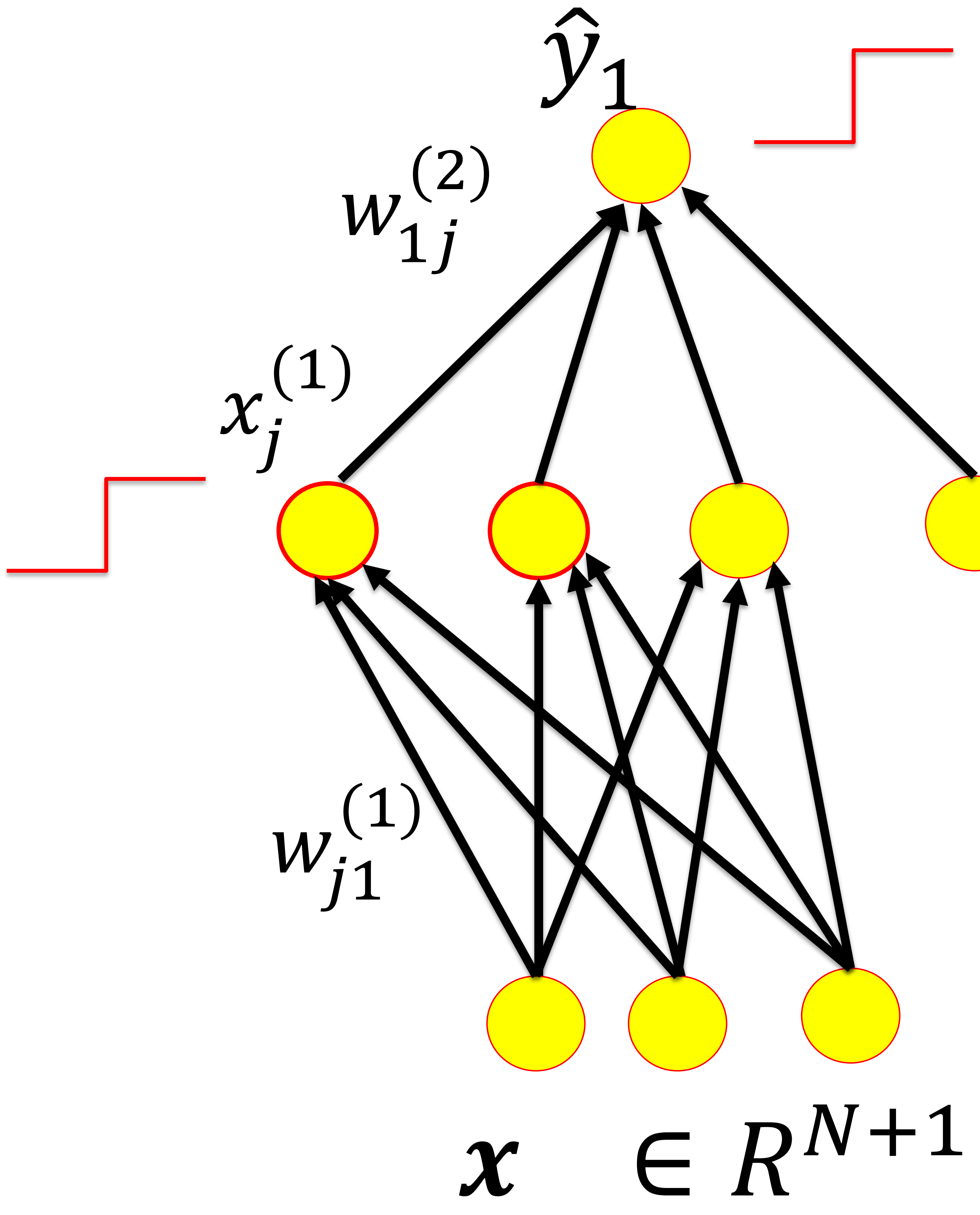
# Preparation for Exercises: Link multilayer networks to probabilities



# Preparation for Exercises: there are many solutions!!!!



**QUIZ: Modern Neural Networks**

[ ]  piecewise linear units should be used in all layers

[ ]  piecewise linear units should be used in the hidden layers

[ ]  softmax unit should be used for exclusive multi-class in an output layer in problems with 1-hot coding

[ ] sigmoidal unit should be used for single-class problems

[ ] two-class problems (mutually exclusive) are the same as single-class problems

[ ] multiple-attribute-class problems are treated as multiple-single-class

[ ] In neural nets we can interpret the output as a probability,

$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x})$$

[ ] if we are careful in the model design, we may interpret the output as a probability that the data belongs to the class

# Artificial Neural Networks: Lecture 3

# Statistical classification by deep networks

Wulfram Gerstner

EPFL, Lausanne, Switzerland

**Objectives for today:**

- The cross-entropy error is the optimal loss function for classification tasks
- The sigmoidal (softmax) is the optimal output unit for classification tasks
- Exclusive Multi-class problems use '1-hot coding'
- Under certain conditions we may interpret the output as a probability
- Piecewise linear units are preferable for hidden layers

## Reading for this lecture:

**Bishop 2006**, Ch. 4.2 and 4.3

*Pattern recognition and Machine Learning*

or

**Bishop 1995**, Ch. 6.7 – 6.9

*Neural networks for pattern recognition*

**or**

**Goodfellow et al.,2016** Ch. 5.5, 6.2, and 3.13 of

*Deep Learning*