Artificial Neural Networks: Lecture 3

Wulfram Gerstner
EPFL, Lausanne, Switzerland

Statistical classification by deep networks

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 and 3.13 of

Deep Learning

Artificial Neural Networks

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1. Simple perceptrons for classification
2. Backprop and multilayer perceptron
3. Statistical Classification by deep networks ← miniproject1
4. Deep learning: TODAY
   regularization and tricks of the trade
5. Complements to deep learning
6. Sequence predictions and LSTMs ← miniproject2
7. Convolutional networks
8. Reinforcement learning1: TD learning
9. Reinforcement learning2: SARSA ← miniproject3
10. Reinforcement learning3: Policy Gradient
11. Deep Reinforcement learning
12. Applications

miniproject1

Handout TODAY

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

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Review: Data base for Supervised learning (single output)

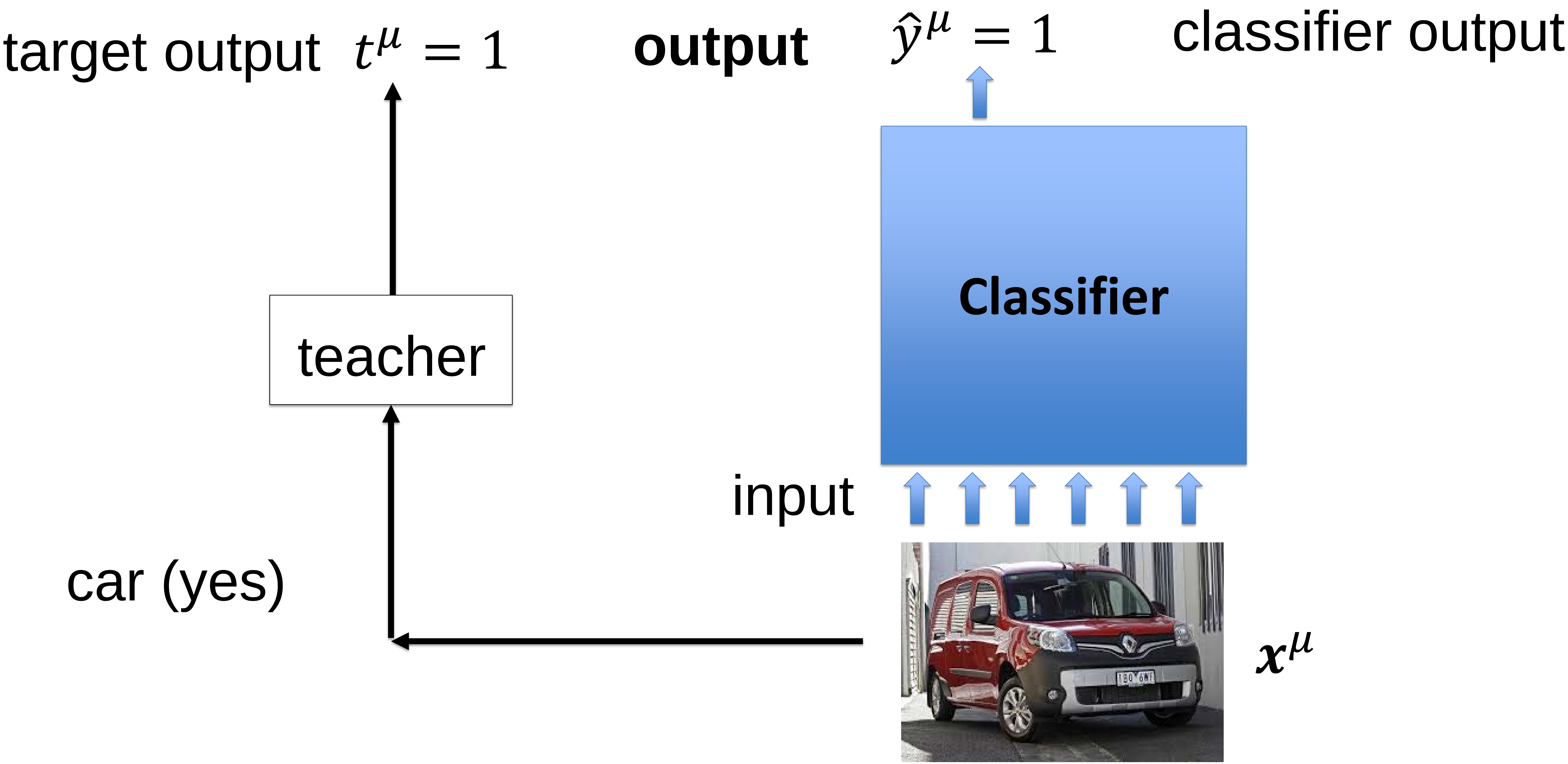
P data points $\{ \quad (\boldsymbol{x}^\mu, t^\mu) \quad , \qquad 1 \leq \mu \leq P \quad \};$

input target output

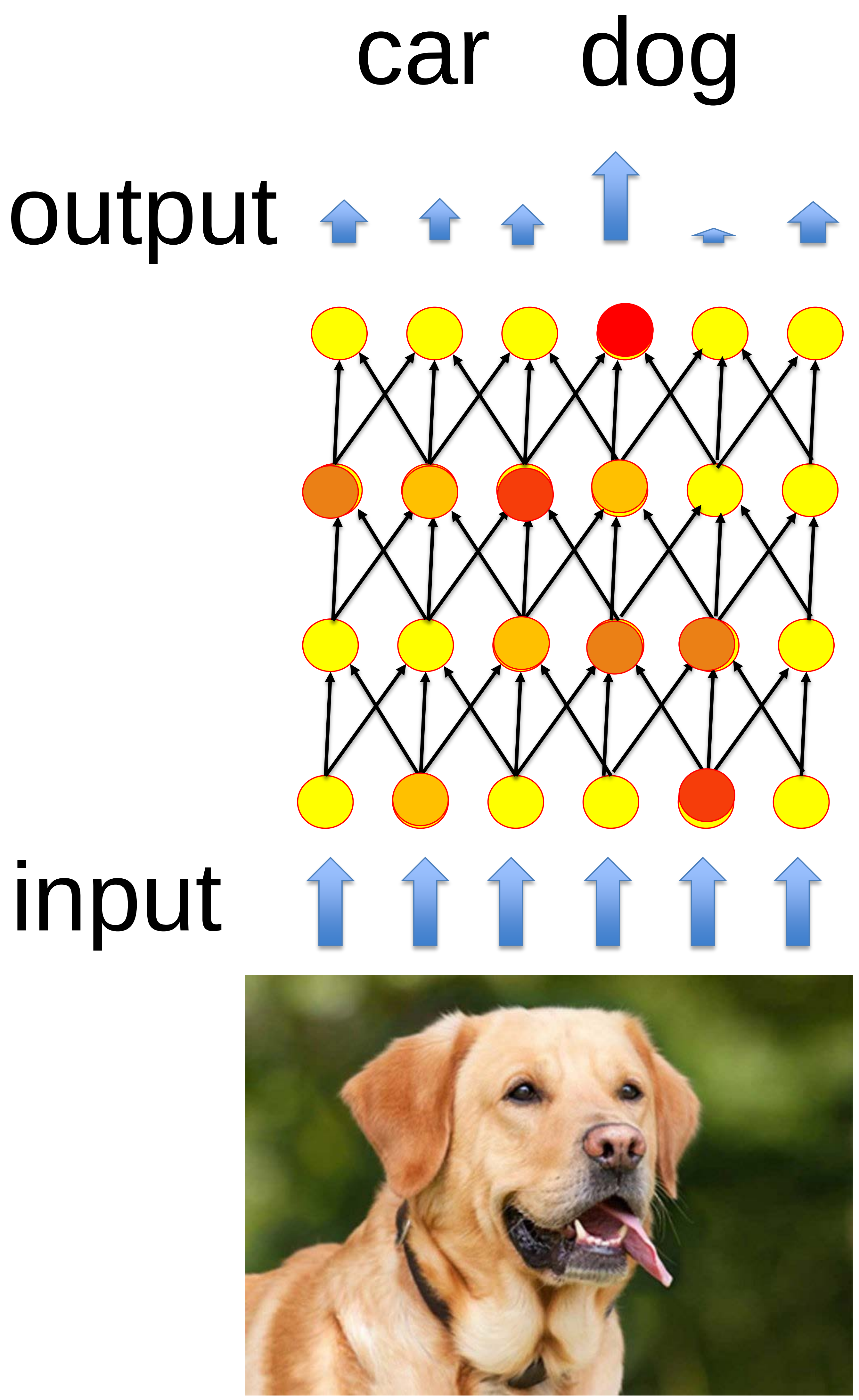
$t^\mu = 1$ car =yes

$t^\mu = 0$ car =no

review: Supervised learning



review: Artificial Neural Networks for classification



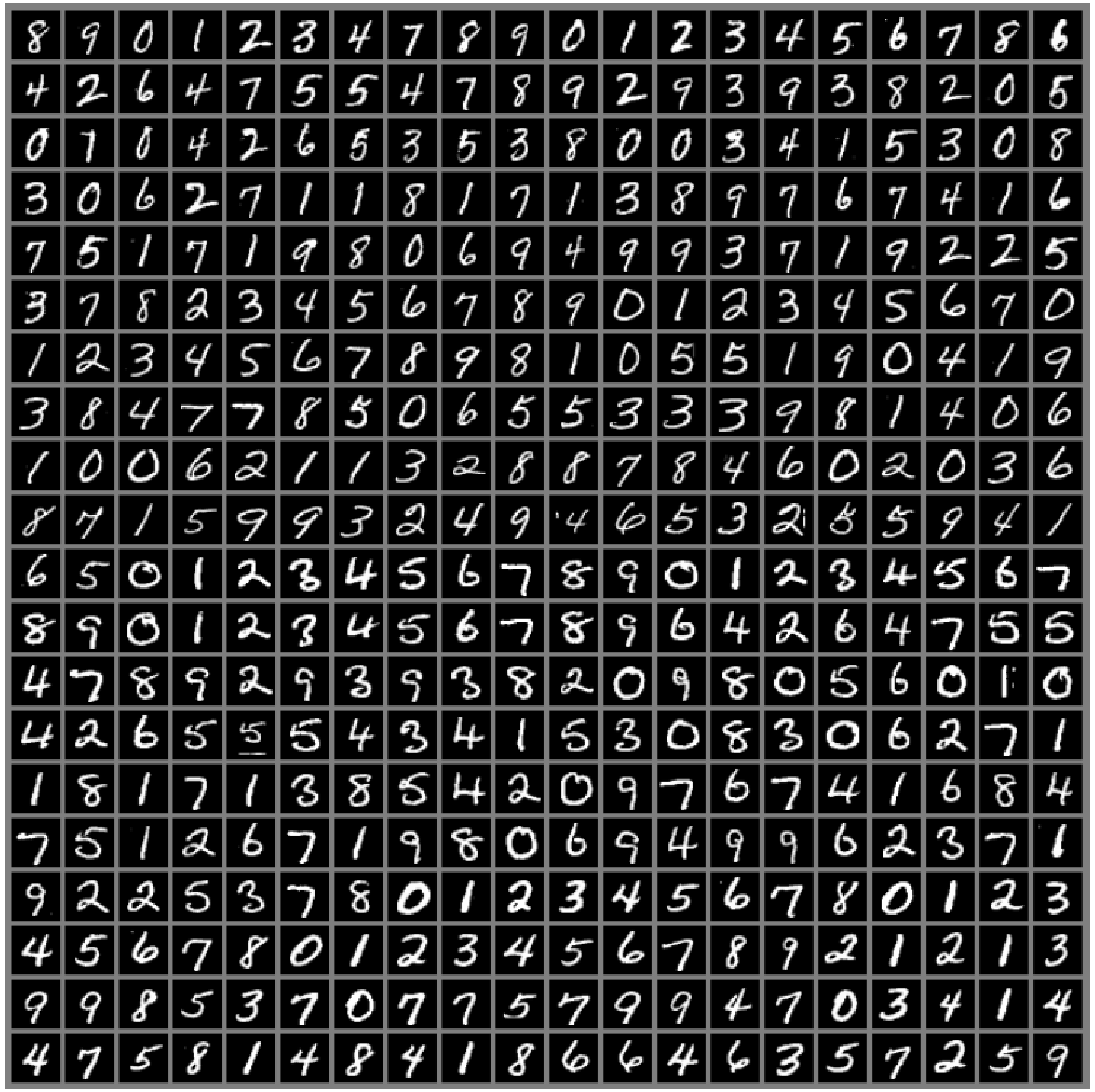
Aim of learning:
Adjust connections such that output is correct (for each input image, **even new ones**)

Review: Example MNIST

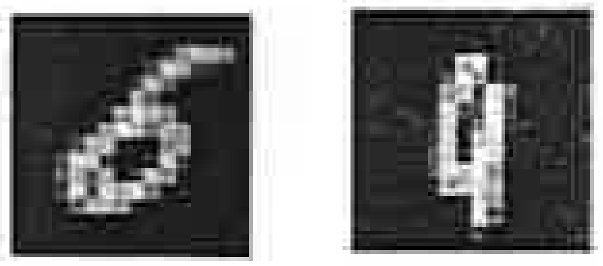
- images 28x28
- Labels: 0, …, 9
- 250 writers
- 60 000 images in training set

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

MNIST data samples



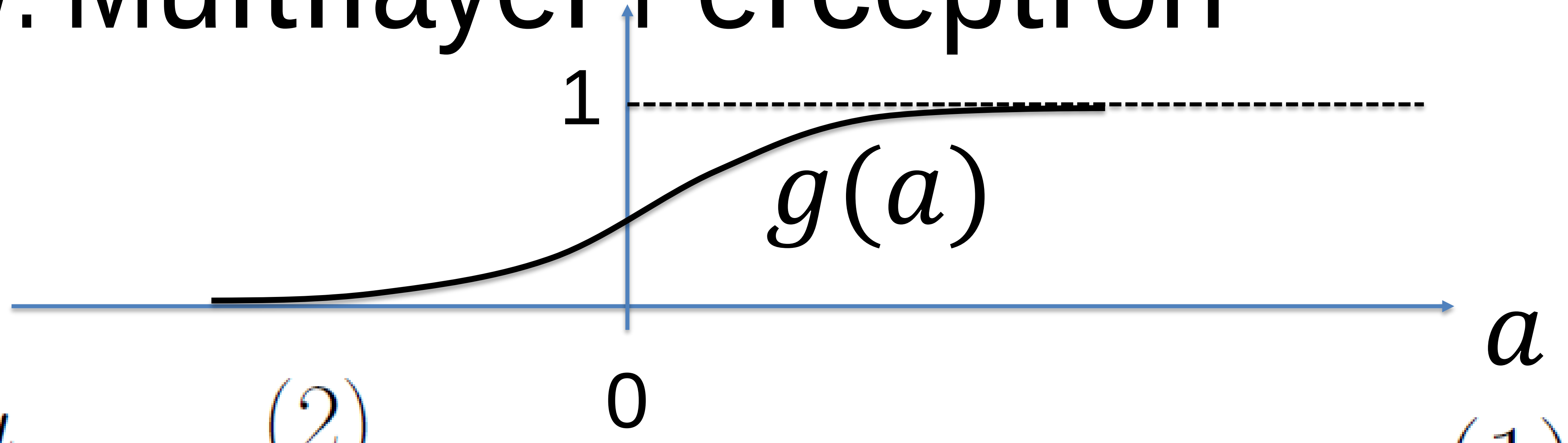
review: data base is noisy



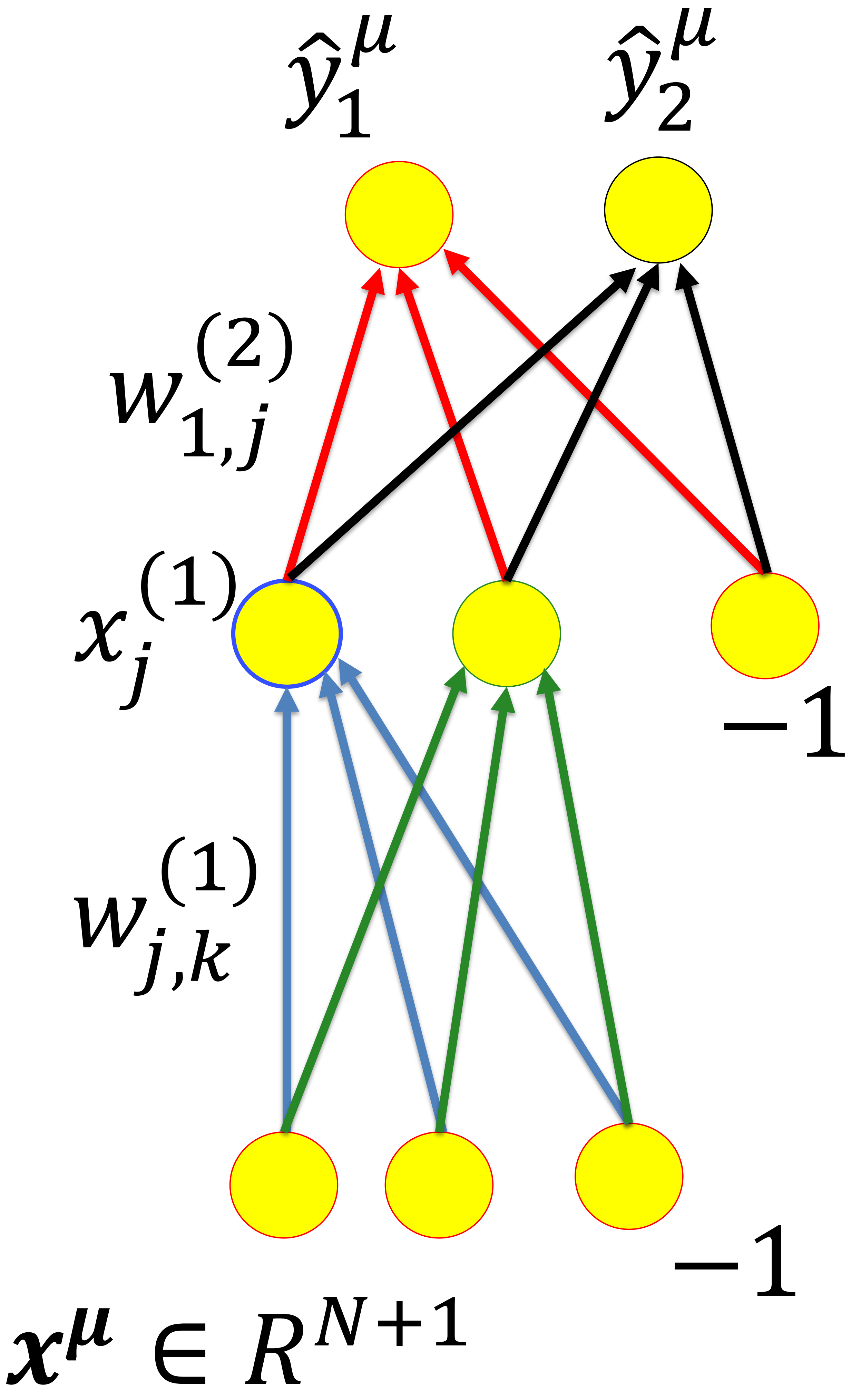
- training data is always noisy
- the future data has different noise

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

Review: Multilayer Perceptron



$$
\begin{aligned}
\hat{y}_i^{\mu} &= x_i^{(2)} && (1)\\
&= g^{(2)}[a_i^{(2)}] && (2)\\
&= g^{(2)}[\sum_j w_{ij}^{(2)} x_j^{(1)}] && (3)\\
&= g^{(2)}[\sum_j w_{ij}^{(2)} g^{(1)}(a_j^{(1)})] && (4)\\
&= g^{(2)}[\sum_j w_{ij}^{(2)} g^{(1)}(\sum_k w_{jk}^{(1)} x_k^{\mu})] && (5)
\end{aligned}
$$



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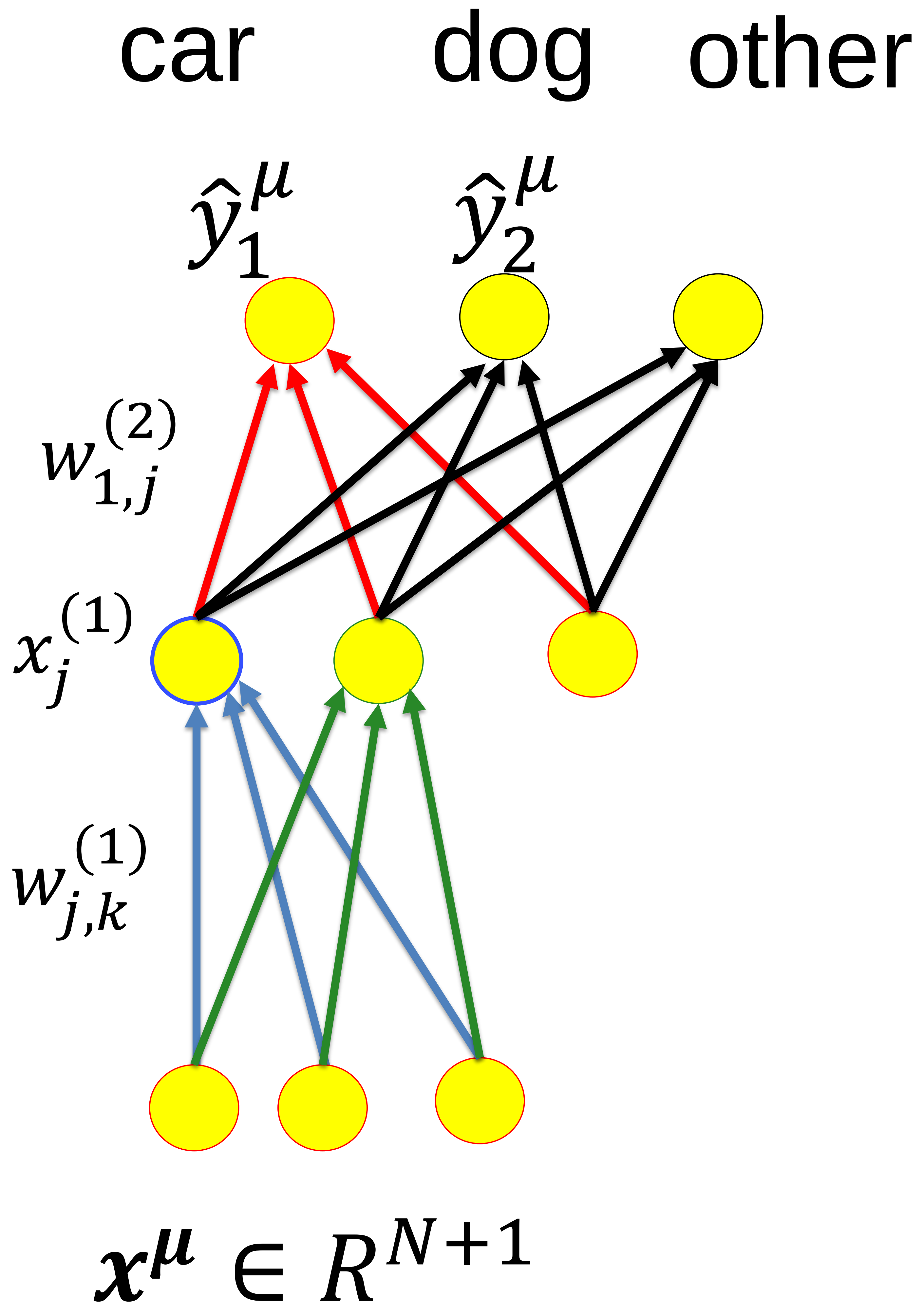
Statistical Classification by Deep Networks

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

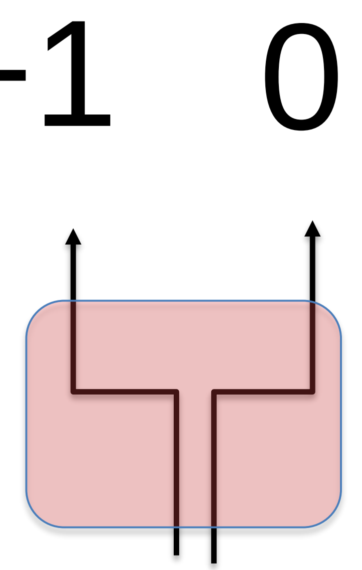


$\hat{y}_k^{\boldsymbol{\mu}} = \mathrm{P}(C_k|\boldsymbol{x}^{\boldsymbol{\mu}})$ pattern from data base

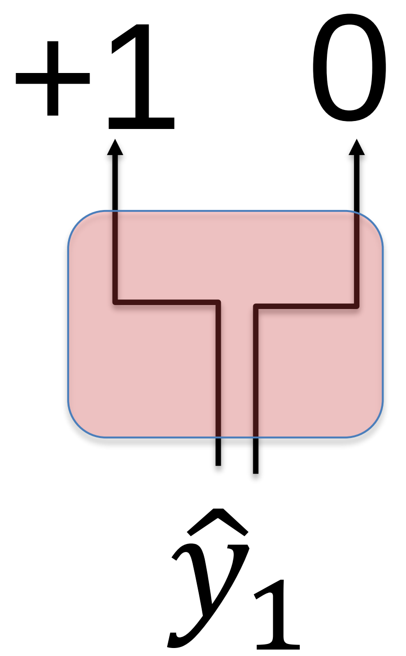
$\hat{y}_k = \mathrm{P}(C_k|\boldsymbol{x} \quad)$ arbitrary novel pattern

1. The statistical view: single class

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

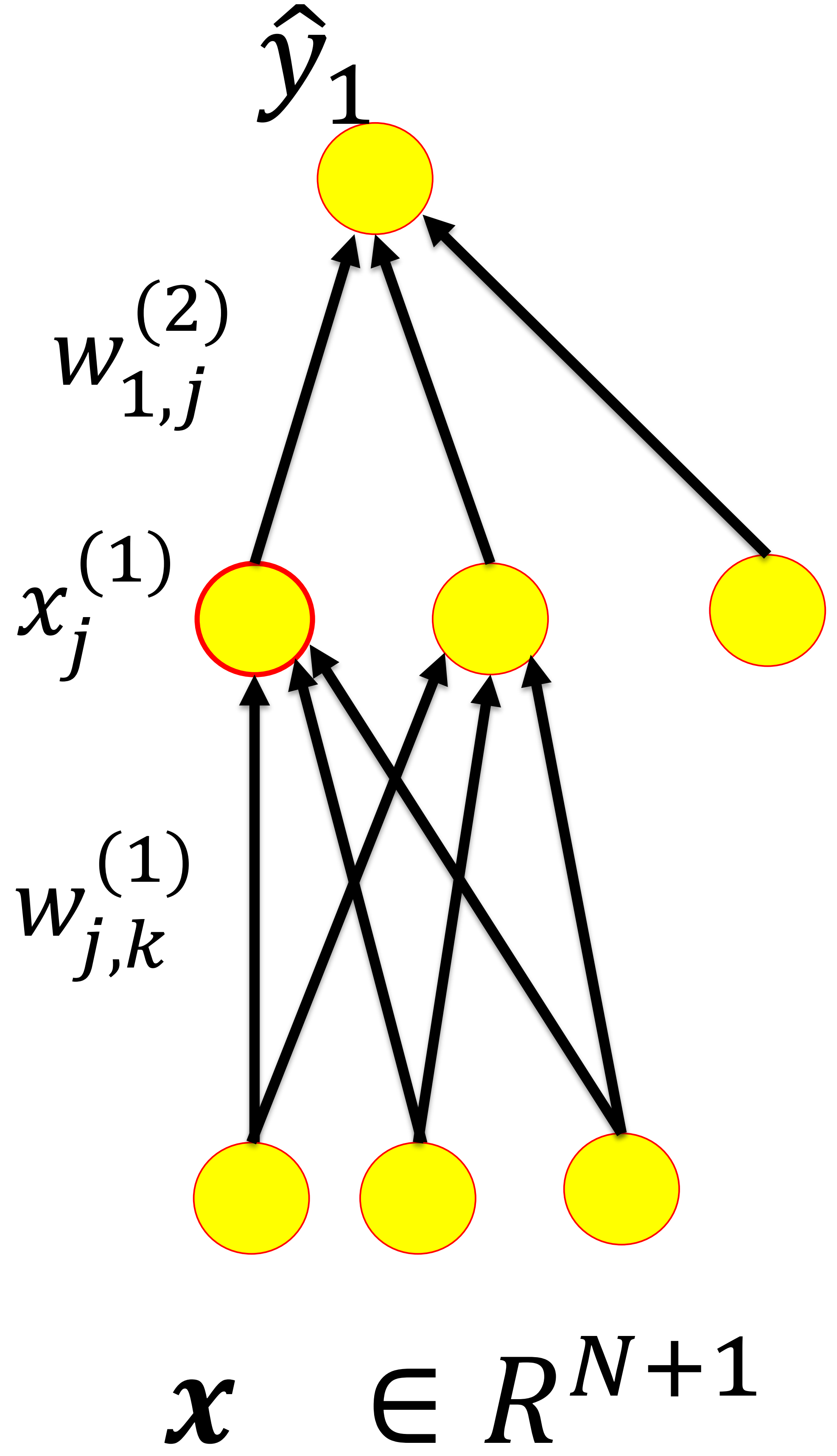


Take the output $\hat{y}_1$ and generate predicted labels $\hat{t}_1$ probabilistically



→ 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



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Statistical Classification by Deep Networks

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

2. The likelihood of data under a model

Overall aim:

What is the likelihood that my set of P data points

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

could have been generated by my model?

2. The likelihood of data under a model

Detour:

forget about labeled data, and just think of input patterns

What is the likelihood that a set of P data points

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

could have been generated by my model?

2. Example: Gaussian distribution

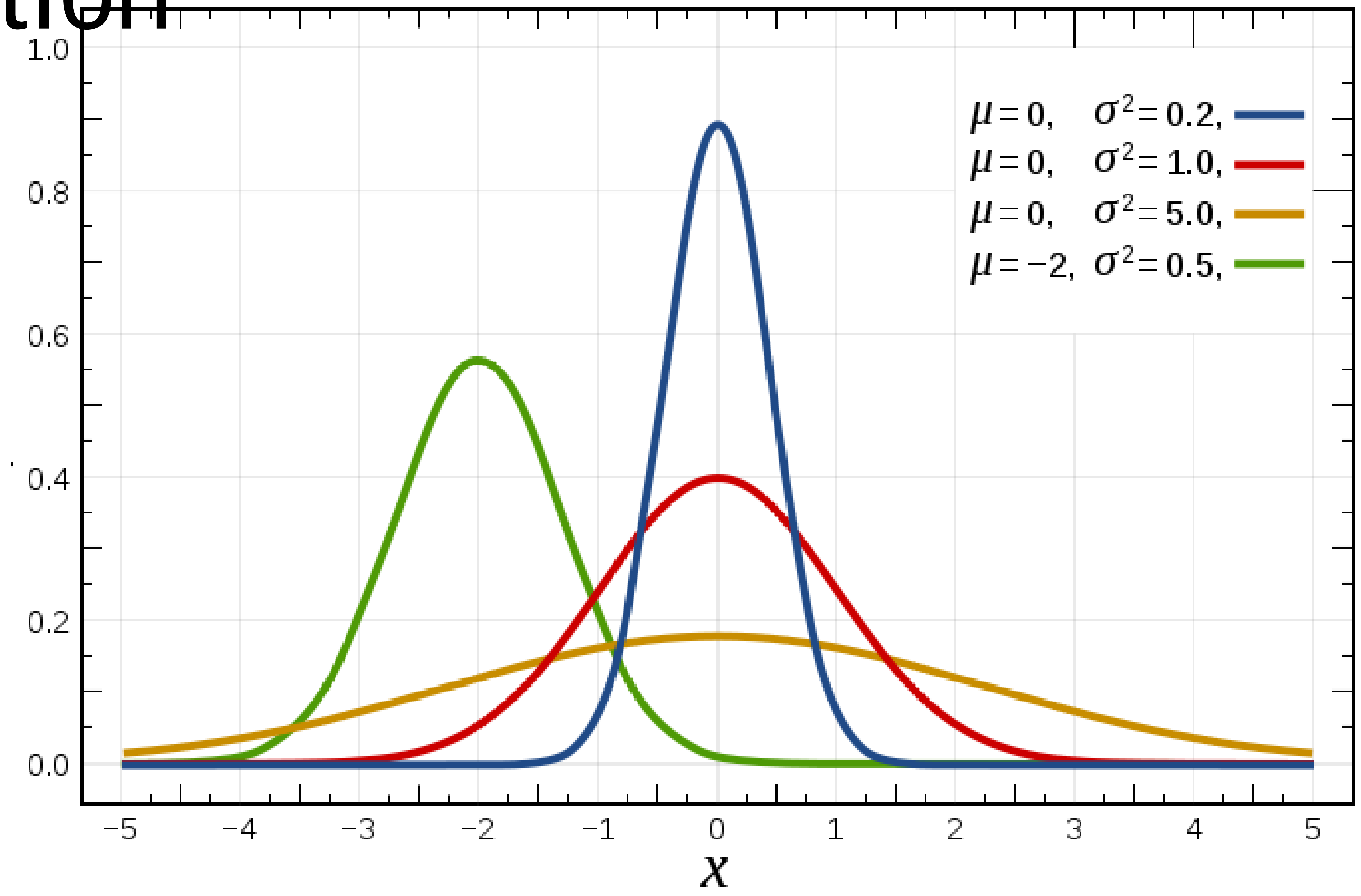
$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} exp\left\{\frac{-(x-\mu)^2}{2\sigma^2}\right\}_1$$

this depends on 2 parameters

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

center

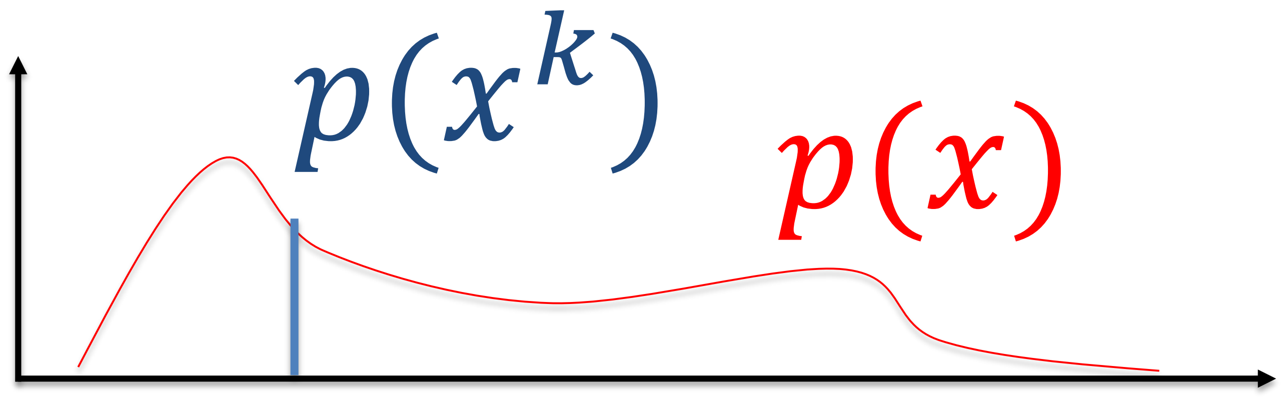
width



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

2. Random Data Generation Process

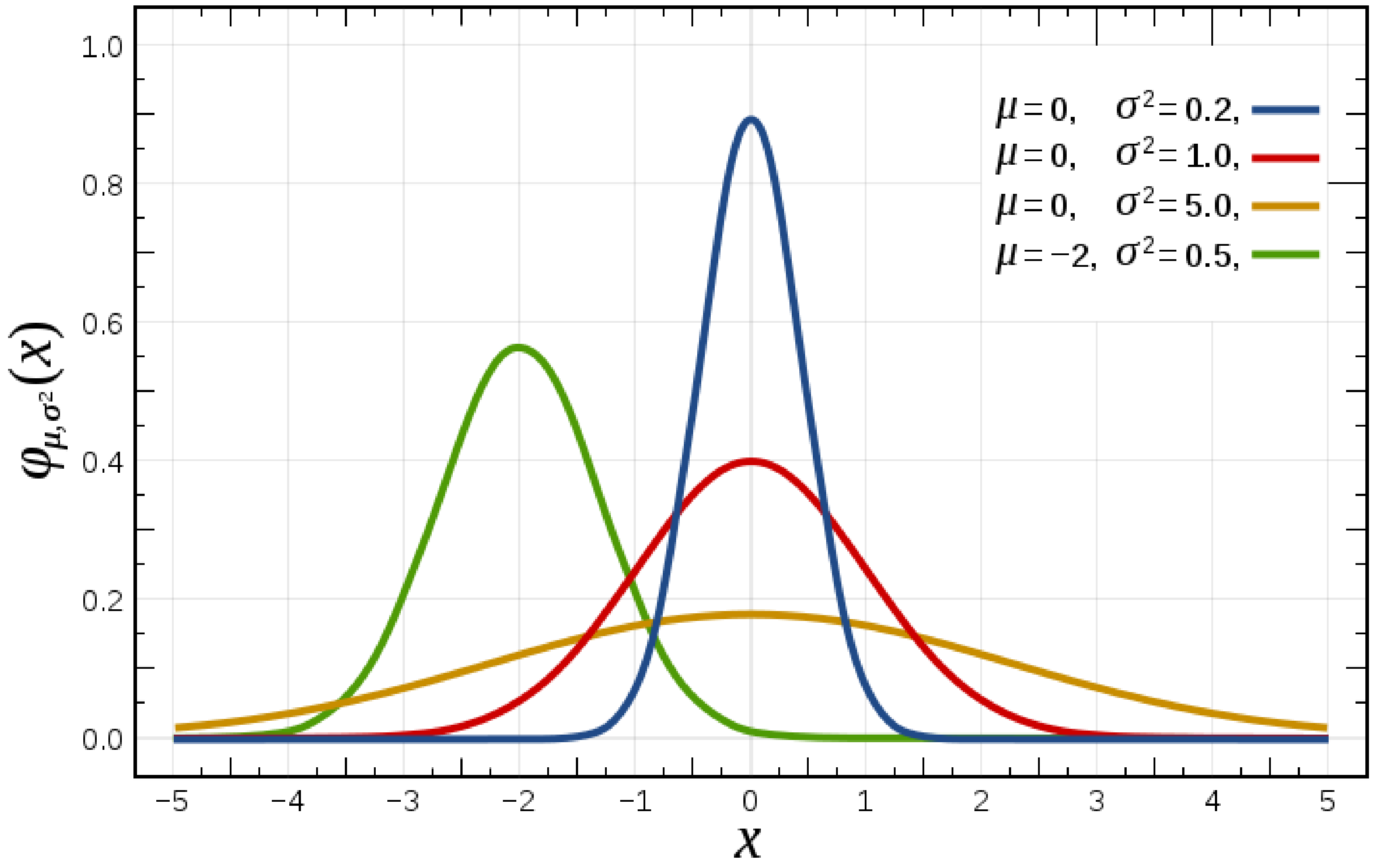
Likelihood that a random data generation process draws one sample k with value x^k is $p(x^k)$



Example: for the specific case of the Gaussian

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

Blackboard 1:
Likelihood of P data points



Blackboard 1:

derive Likelihood function

2. Likelihood function (beyond Gaussian)

Suppose the likelihood for generating a data point $\boldsymbol{x}^k$ is

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

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)

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

BUT this likelihood depends on the parameters of my model

$$p_{model}(\boldsymbol{X}) = p_{model}\left(\boldsymbol{X} \middle| \left\{w_{1,} w_{2,} \ldots w_{n,}\right\}\right)$$

parameters

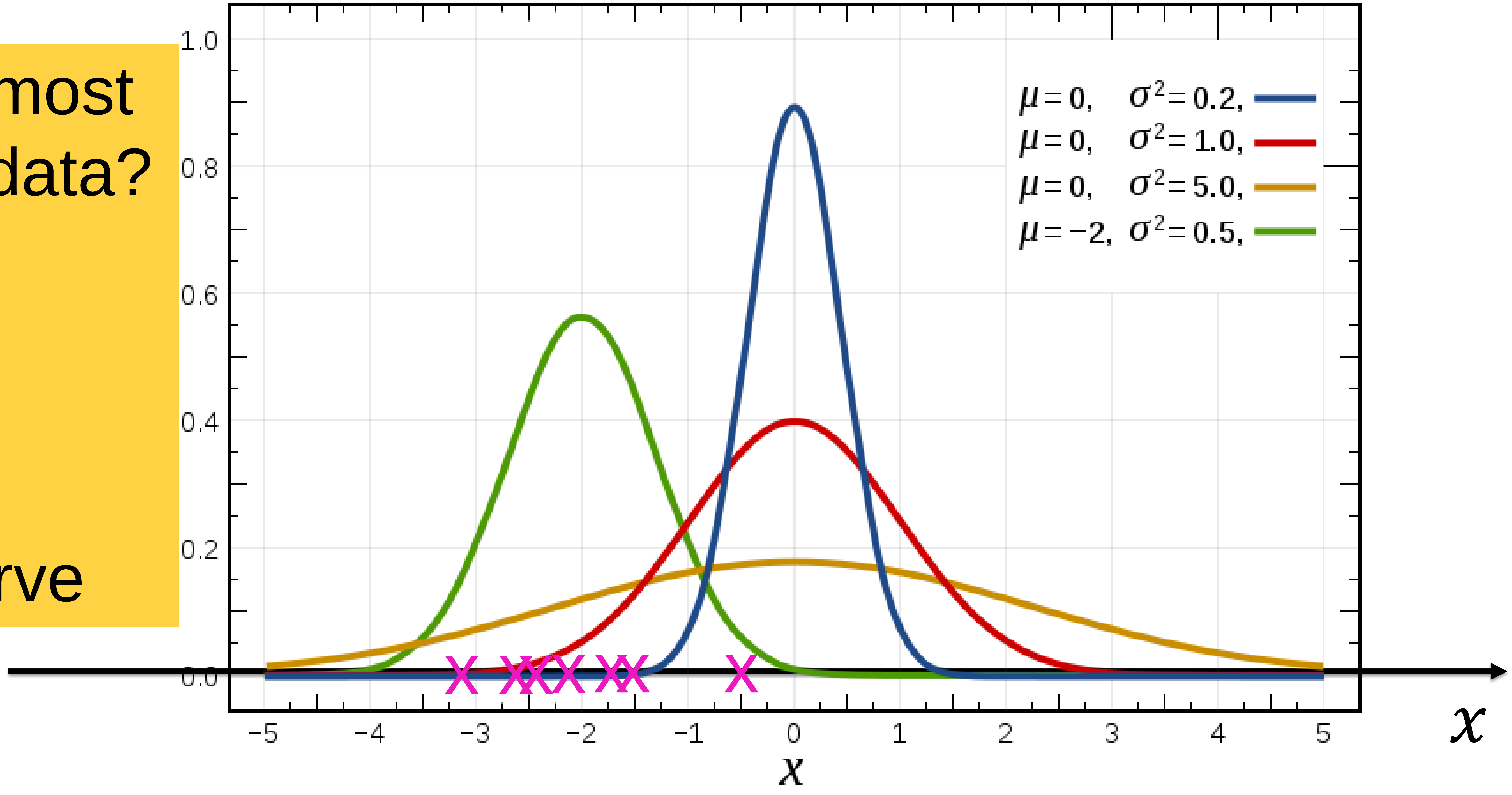
Choose the parameters such that the likelihood is maximal!

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

$$p_{model}(\boldsymbol{X}) = p_{model}\left(\boldsymbol{X} | \{w_{1,} w_2\}\right)$$

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

Exercise 1 NOW! (8 minutes): you have P data points

Calculate the **optimal choice** of parameter μ:

To do so maximize $p_{model}(\boldsymbol{X})$ with respect to μ

Blackboard 2:

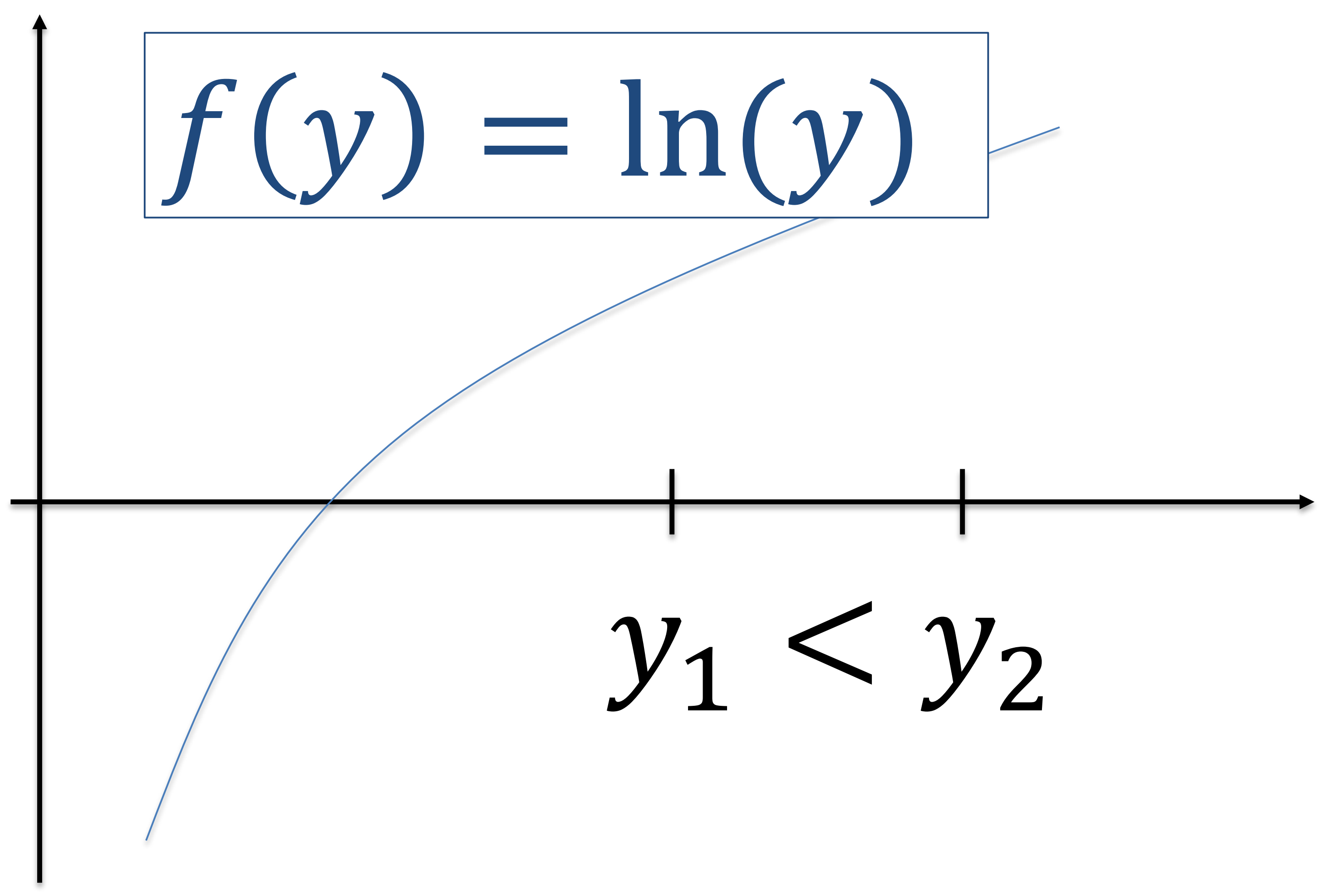
Gaussian: best parameter choice for center

2. Maximum Likelihood (general)

Choose the parameters such that the likelihood

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

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)

Choose the parameters such that the likelihood

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

is maximal is equivalent to maximizing the log-likelihood

$$LL = \ln(p_{model}) = \sum_k ln\ p(\boldsymbol{x}^k)$$

"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)

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**

3. The likelihood of data under a neural network model

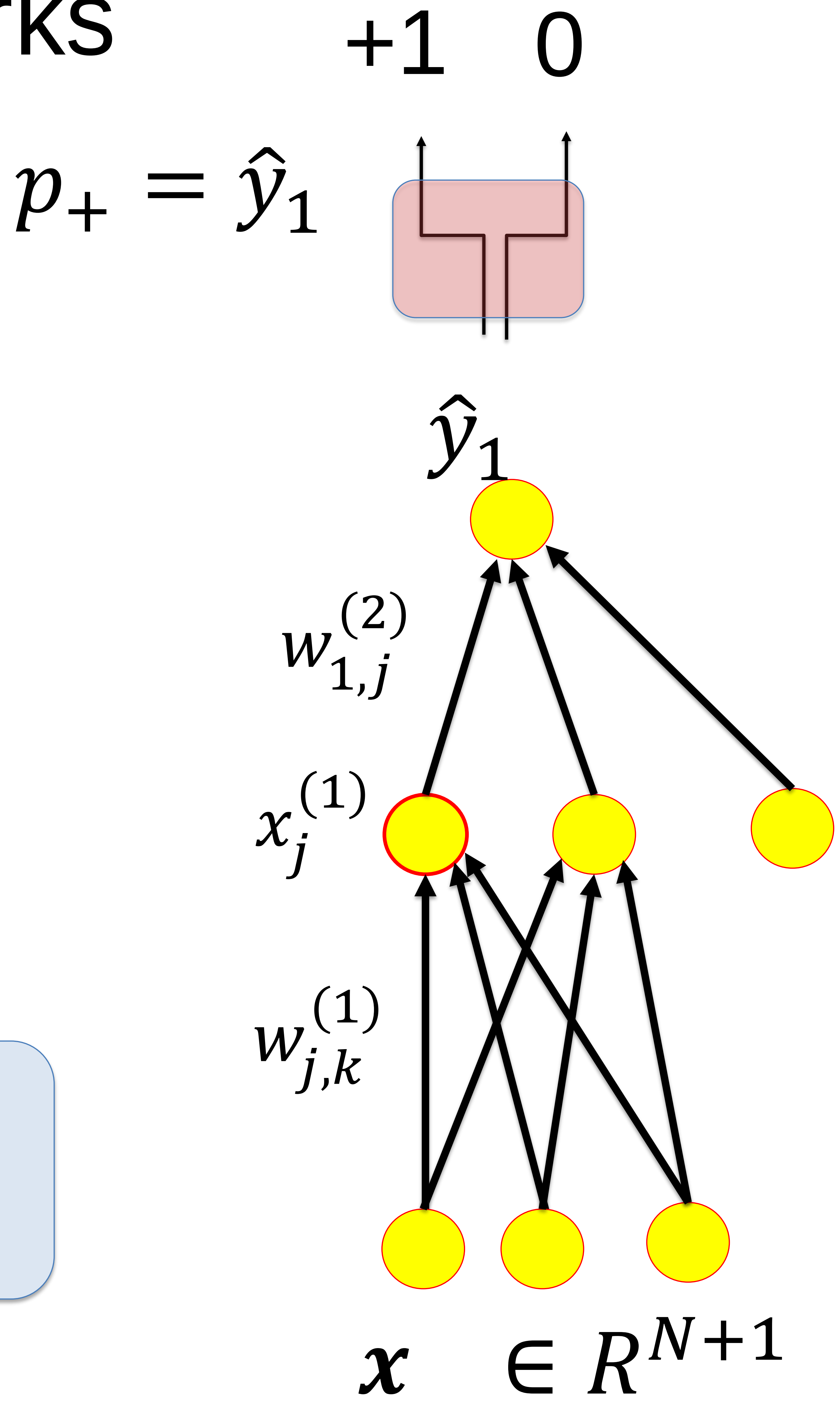
Overall aim:

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

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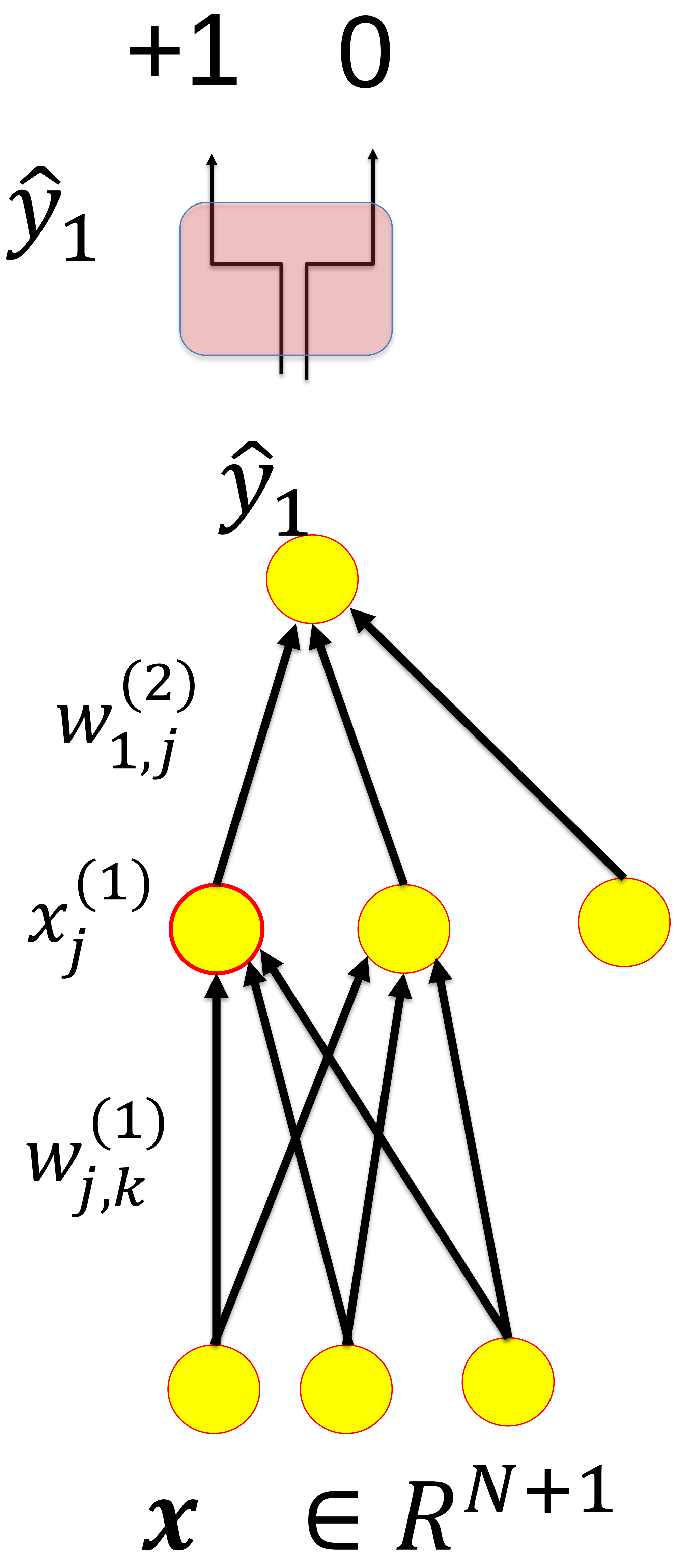
Likelihood of P input-output pairs

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

A **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

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

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Statistical Classification by Deep Networks

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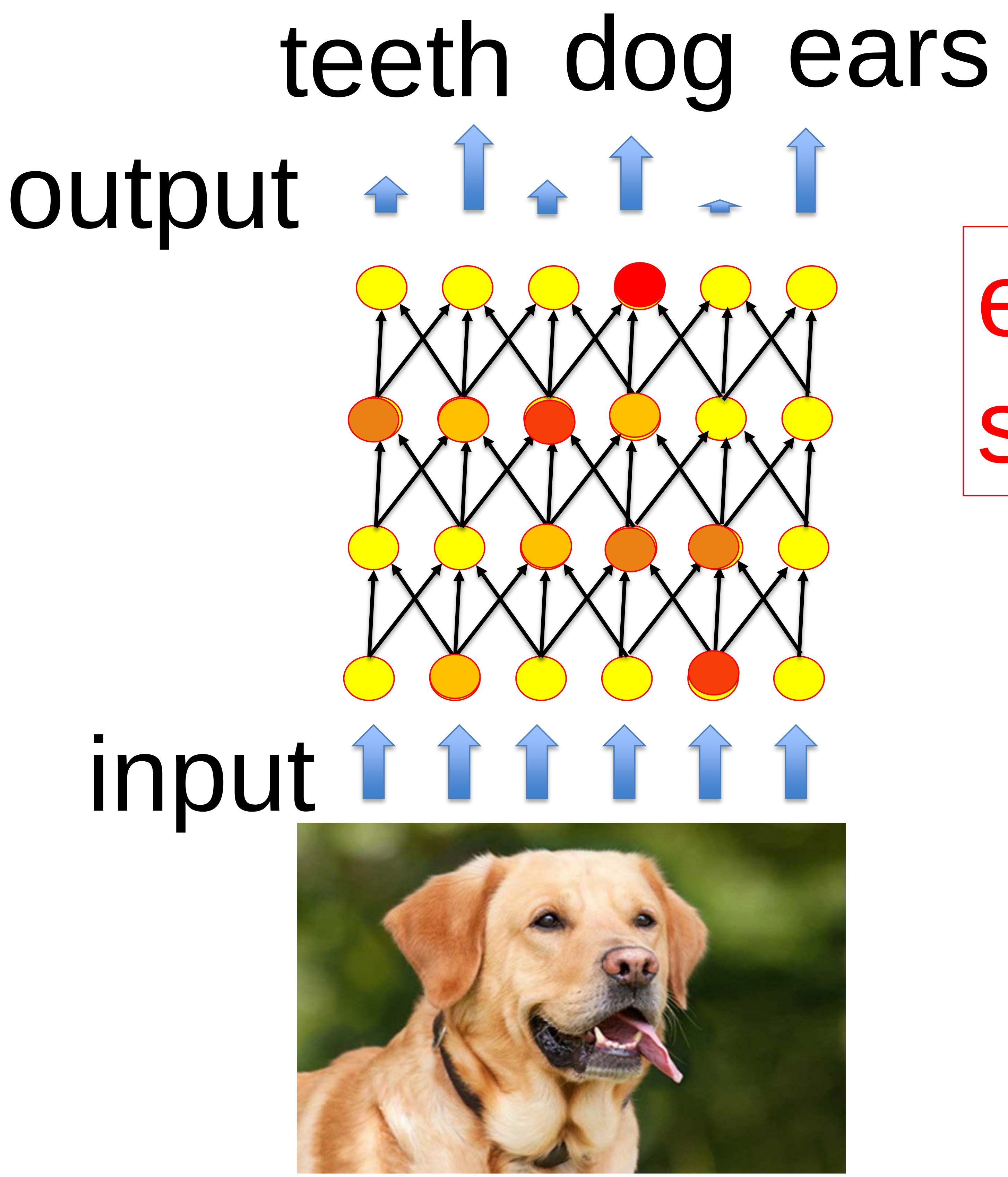
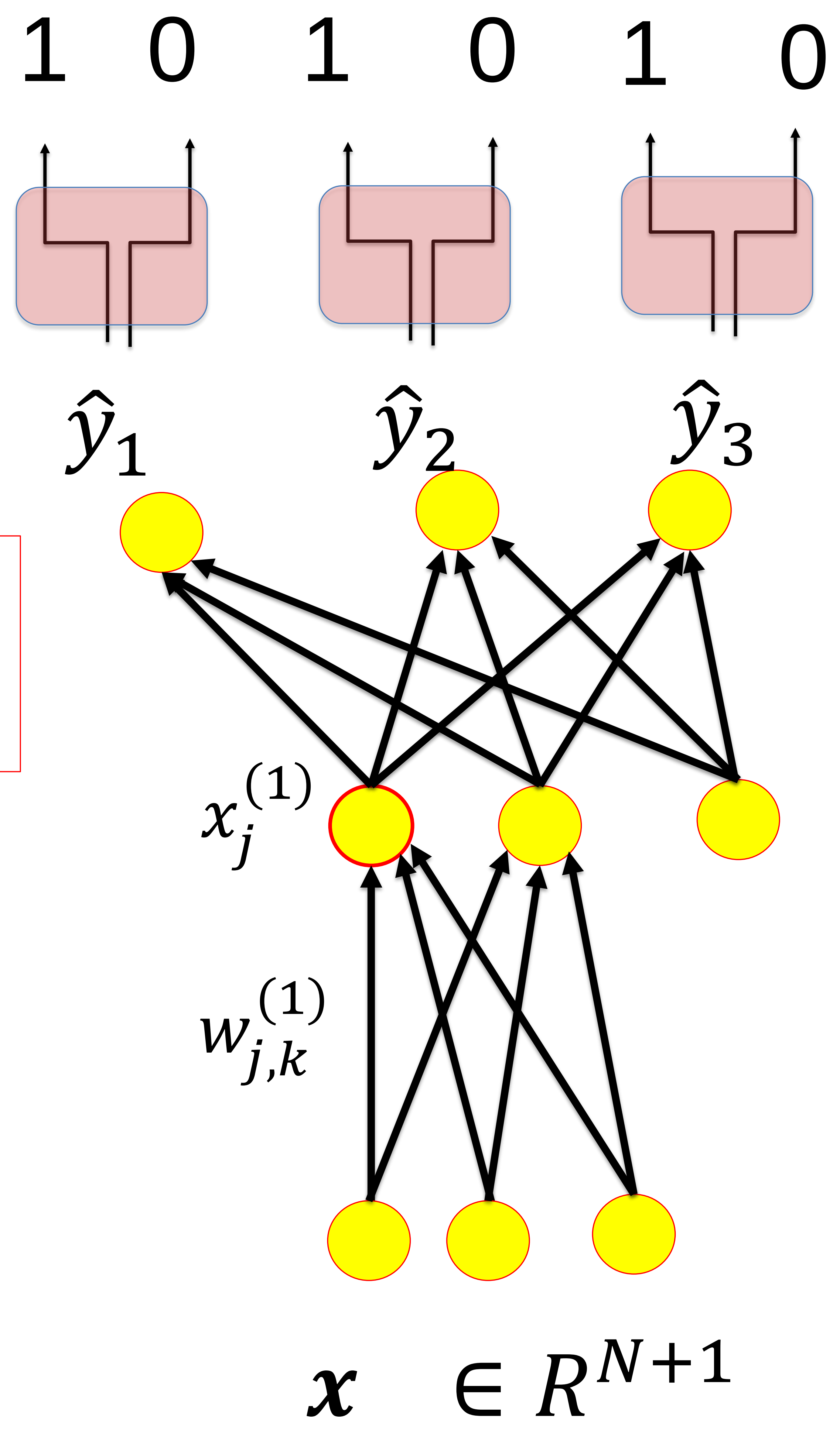
1. The statistical view: generative model
2. The likelihood of data under a model
3. Application to artificial neural networks
4. Multi-class and 1-hot coding

4. Multiple Classes: Multiple attributes

Multiple attributes:



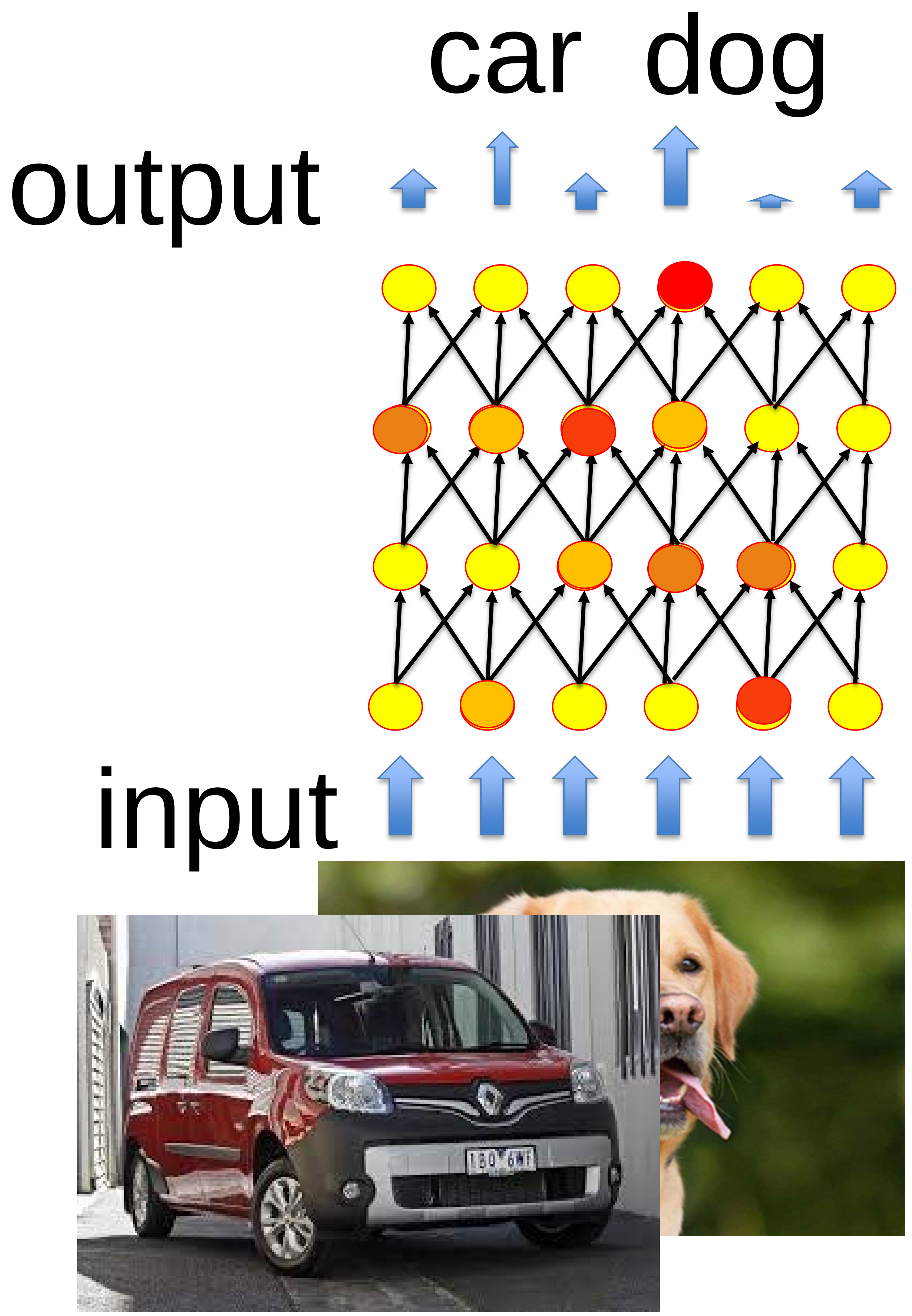
equivalent to several single-class decisions



4. Multiple Classes: Mutuall exclusive classes

mutually exclusive classes

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

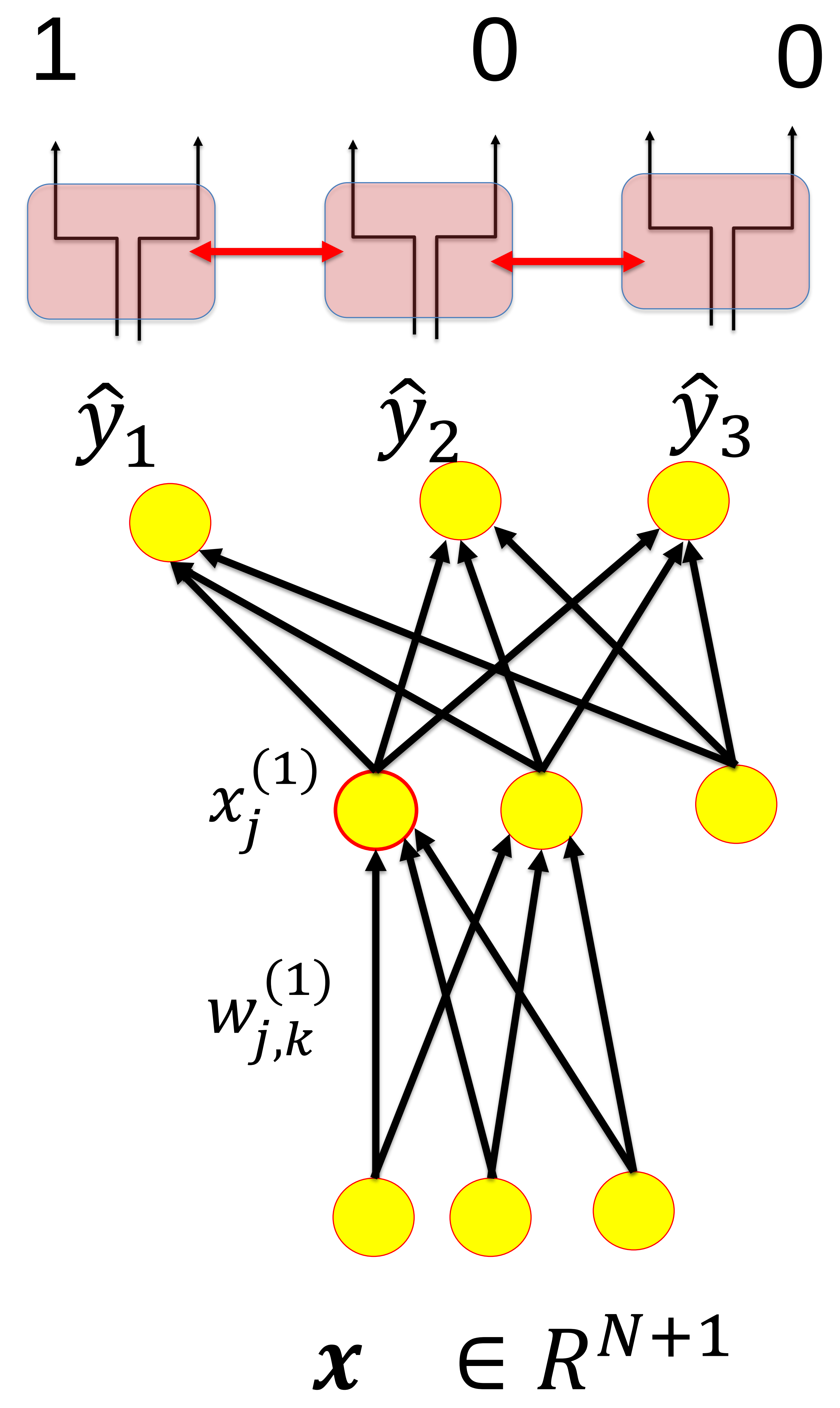


4. Exclusive Multiple Classes

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

1-hot-coding:

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



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

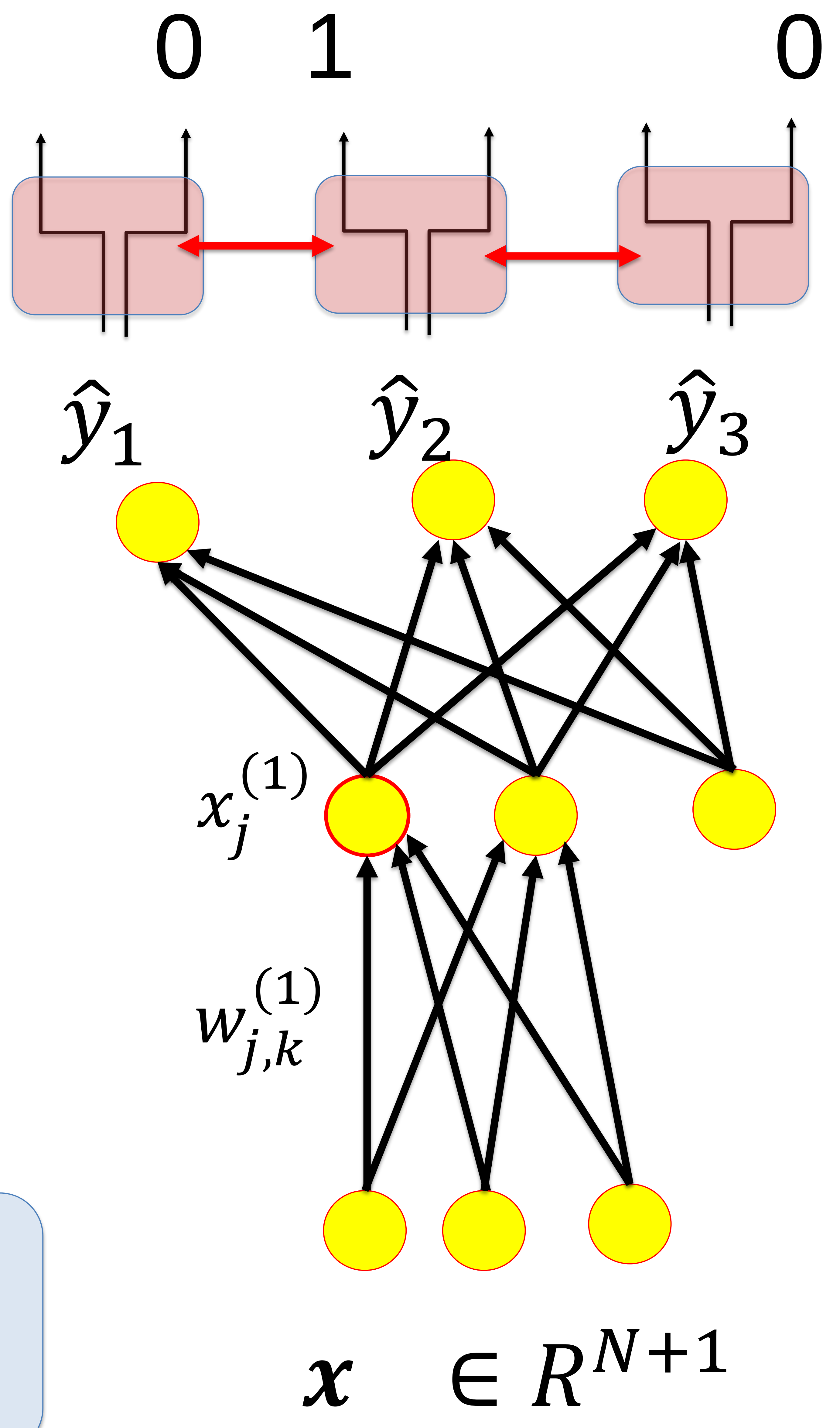
1-hot-coding:

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

Outputs are NOT independent:

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

Blackboard 5:
derive likelihood function



Blackboard 5:

Likelihood of P input-output pairs

4. 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

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

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

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

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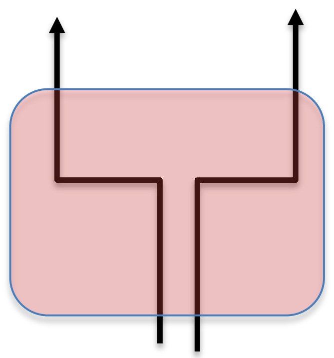
1. The statistical view: generative model
2. The likelihood of data under a model
3. Application to artificial neural networks
4. Multi-class problems
5. **Sigmoidal as a natural output function**

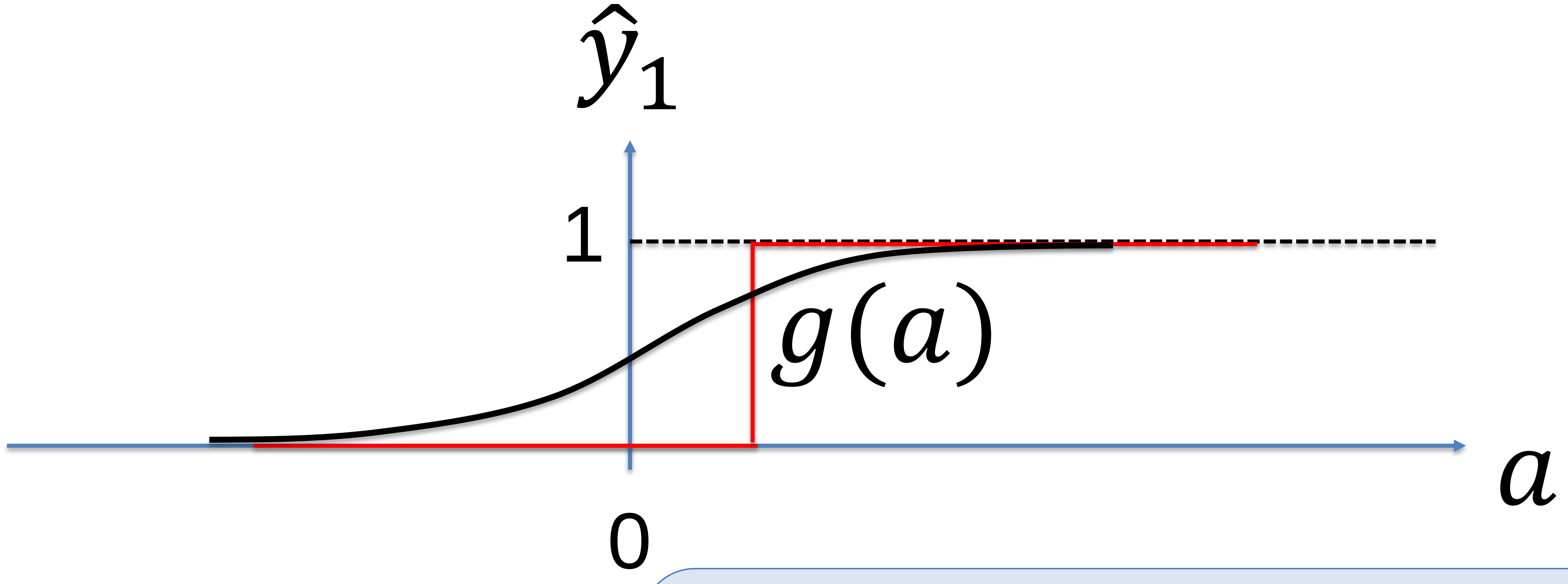
5. Why sigmoidal output ? – single class

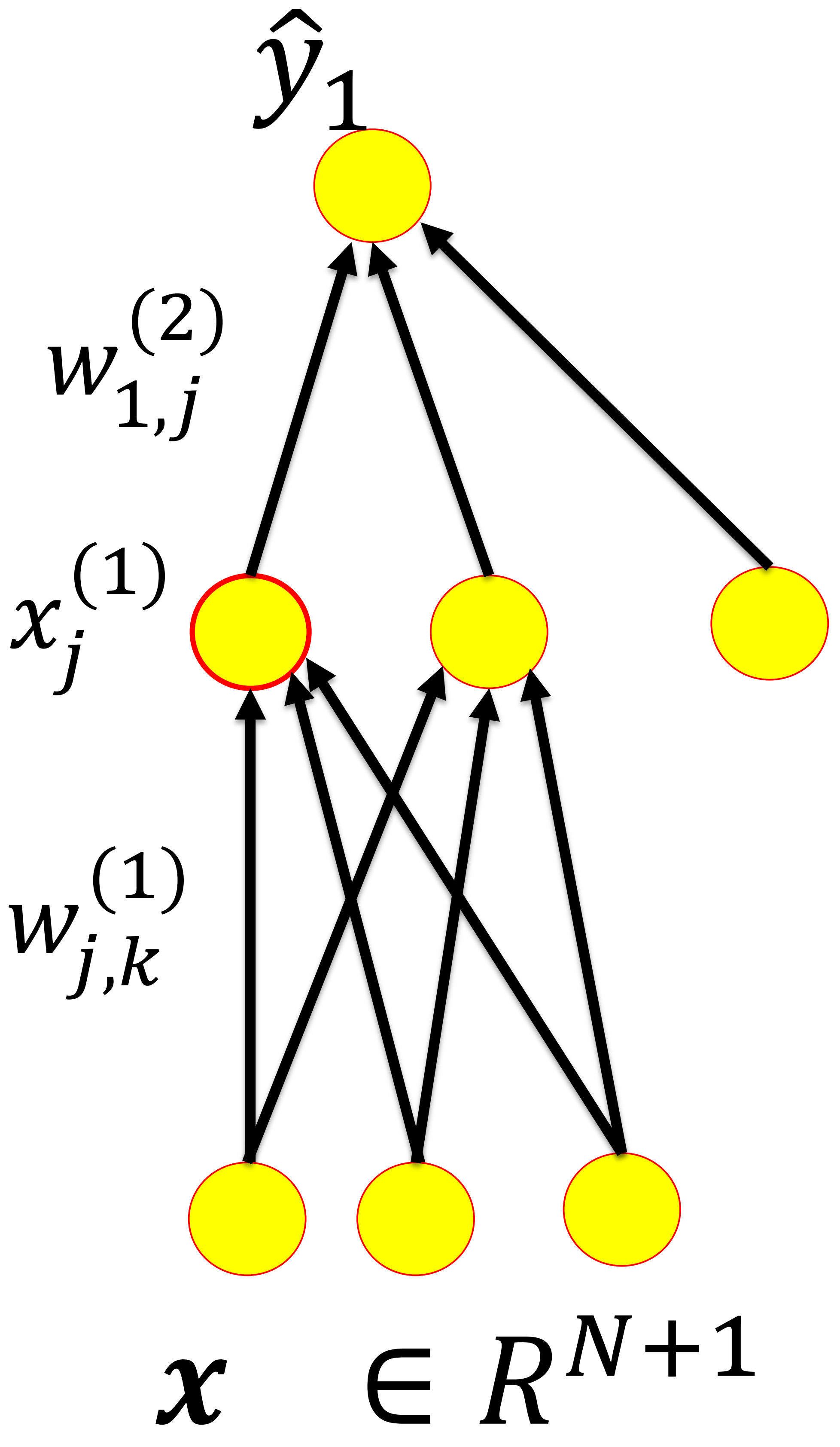
$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

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

Observations (single-class):

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

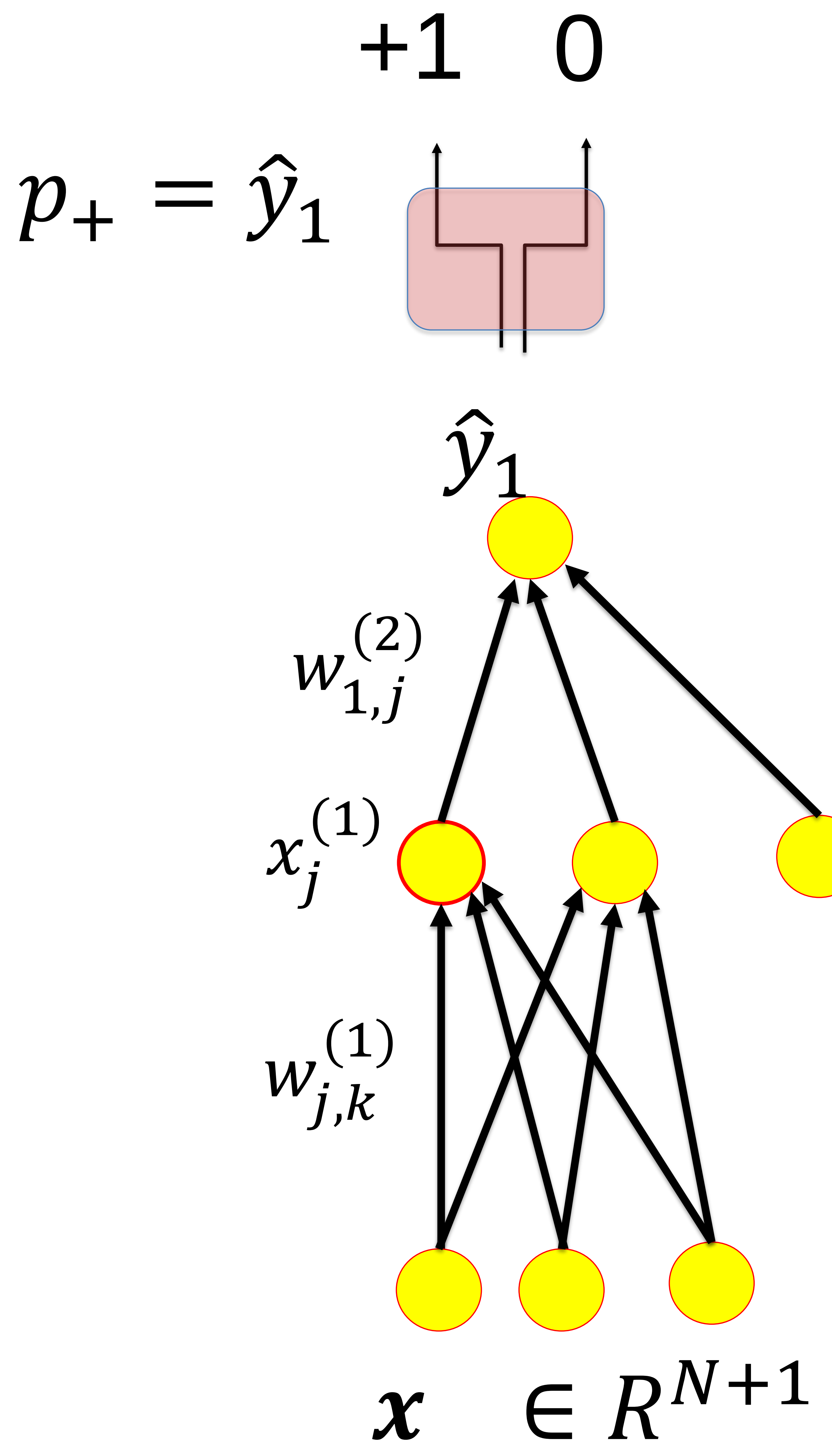




Blackboard 6:

derive optimal sigmoidal

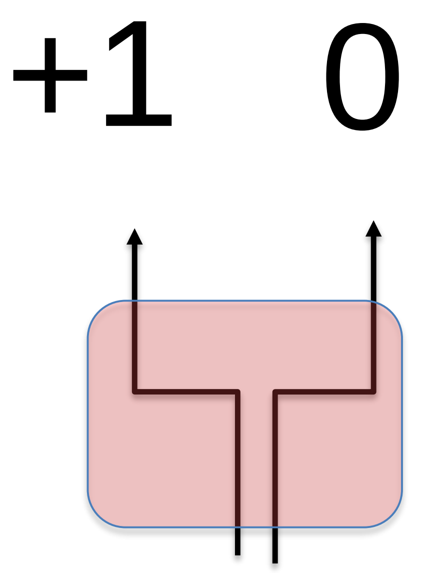
Blackboard 6:
derive optimal sigmoidal



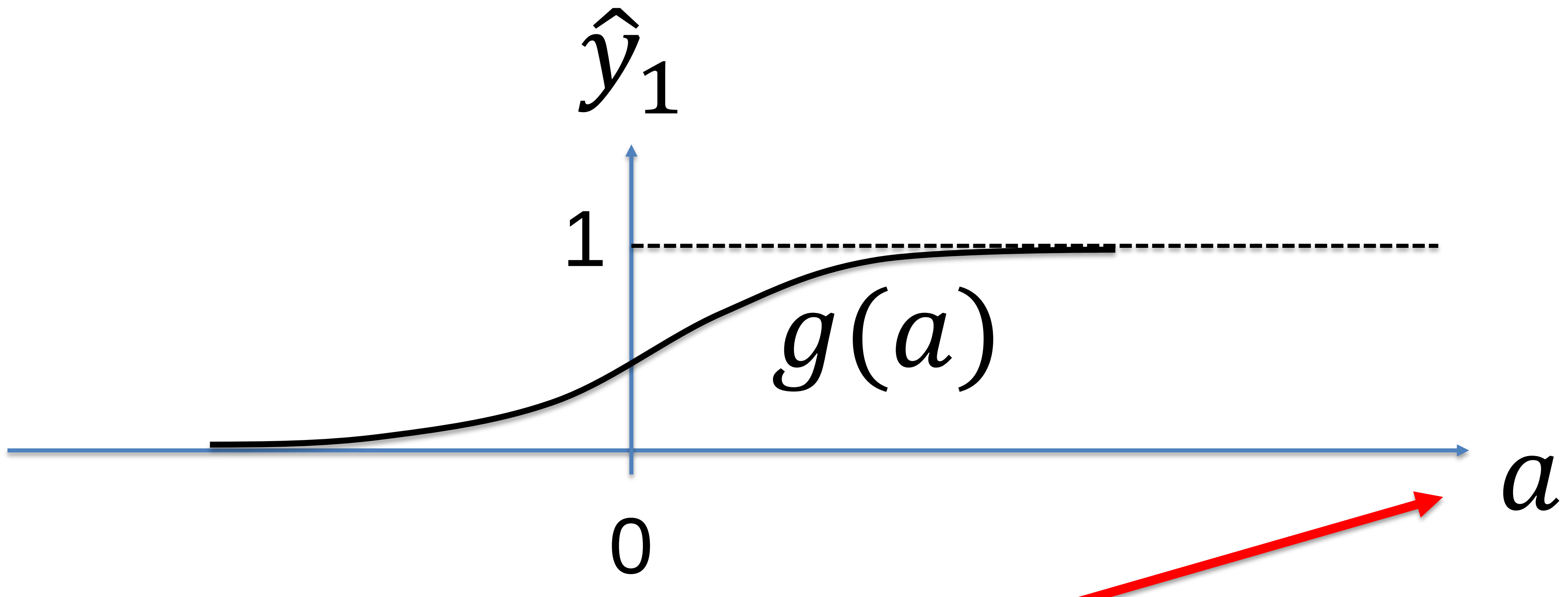
5. Why sigmoidal output ? – single class

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

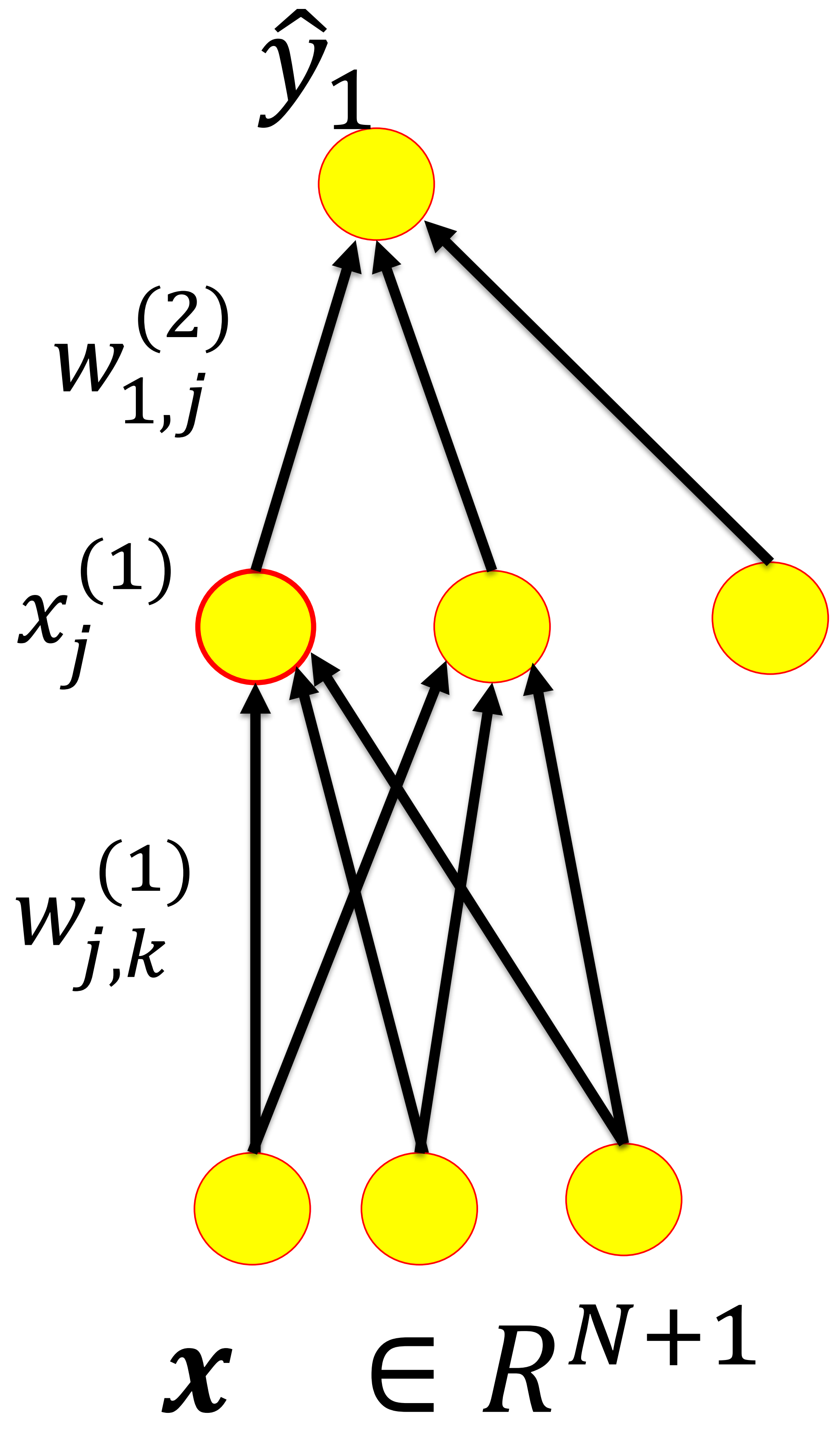
$$p_+ = \hat{y}_1$$



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



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



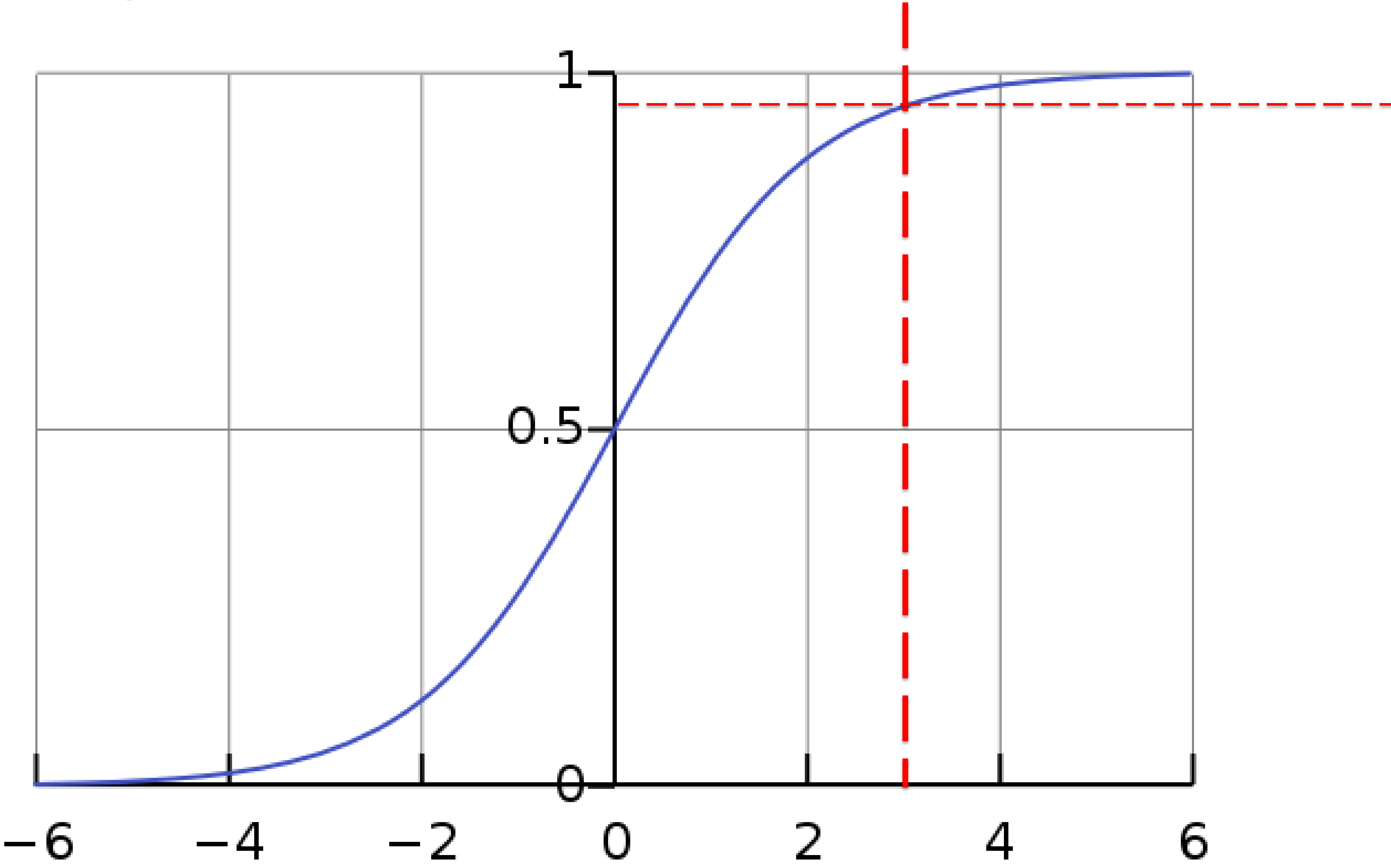
5. sigmoidal output **= logistic function**

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

Rule of thumb:

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

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



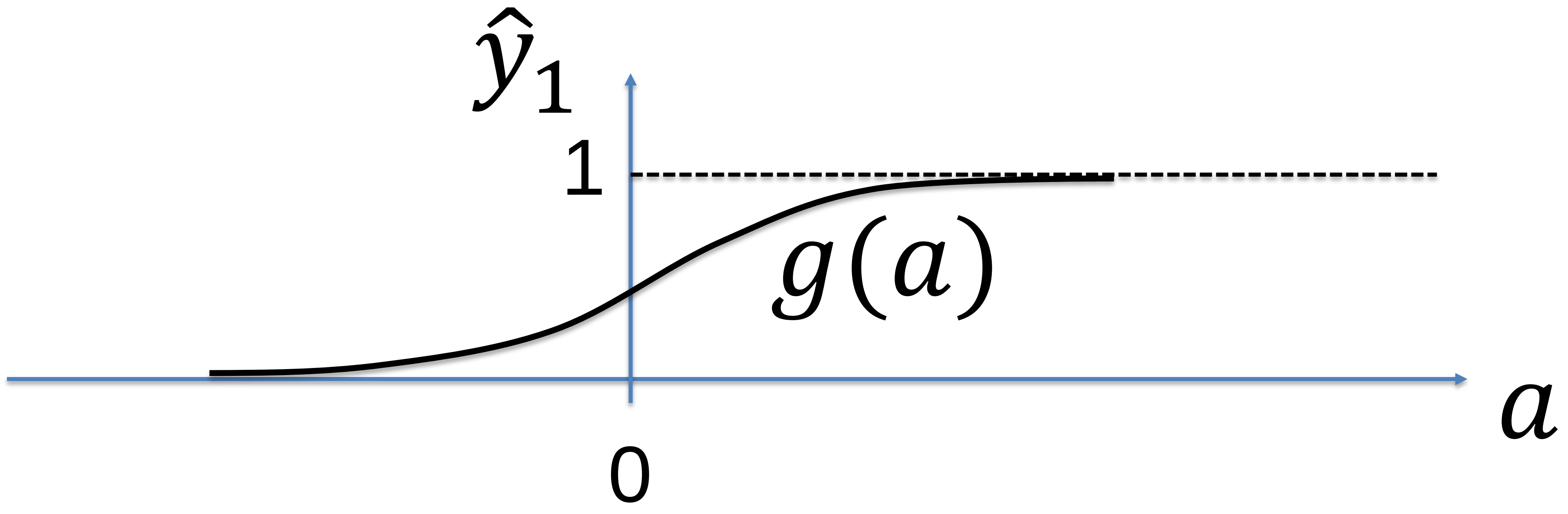
https://en.wikipedia.org/wiki/Logistic_function

5. Why sigmoidal output ?

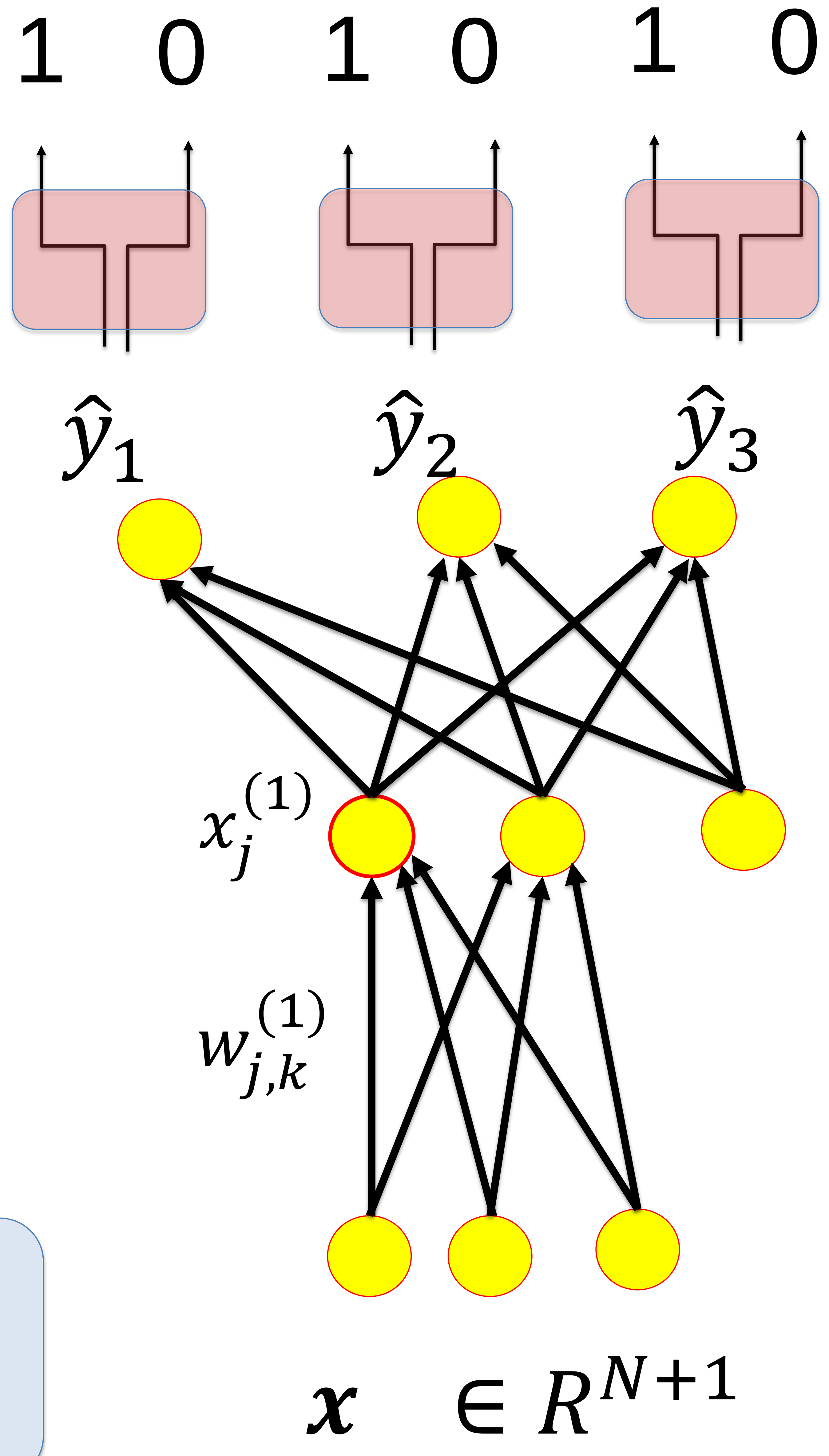
$$\hat{y}_1 = \mathrm{P}(C_1|\boldsymbol{x}) = \boldsymbol{P}(\hat{t}_1 = 1|\boldsymbol{x})$$

Observations (multiple-classes):

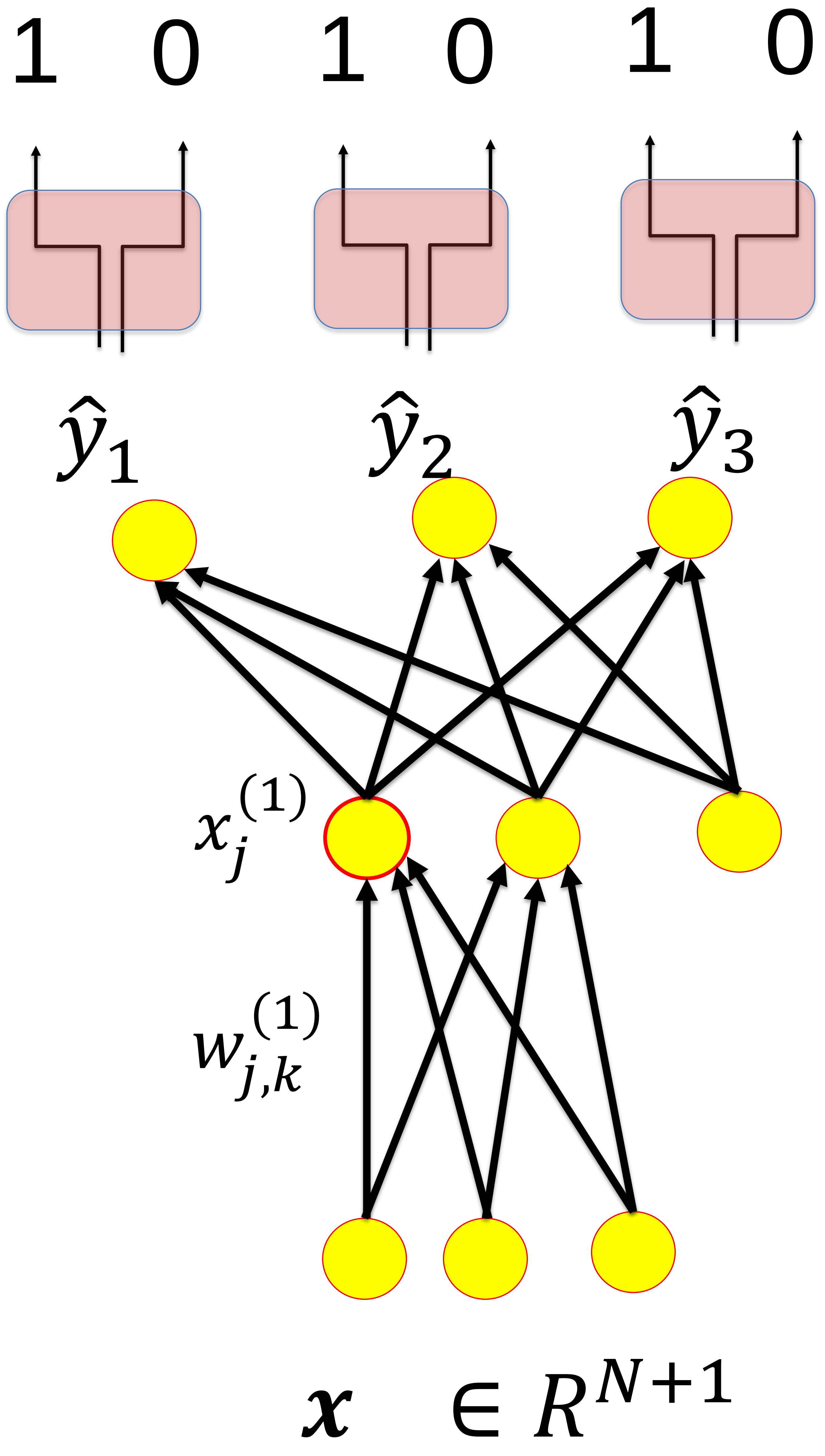
- Probabilities must sum to one!



Blackboard 7:
derive optimal output



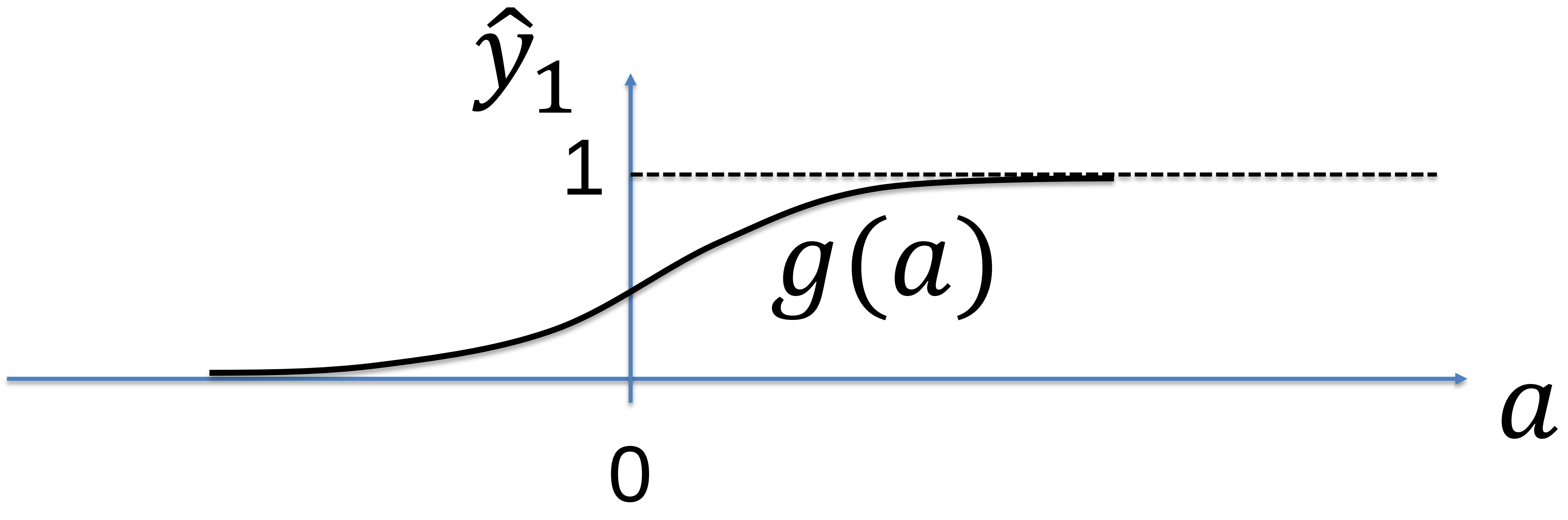
Blackboard 7:
derive optimal output

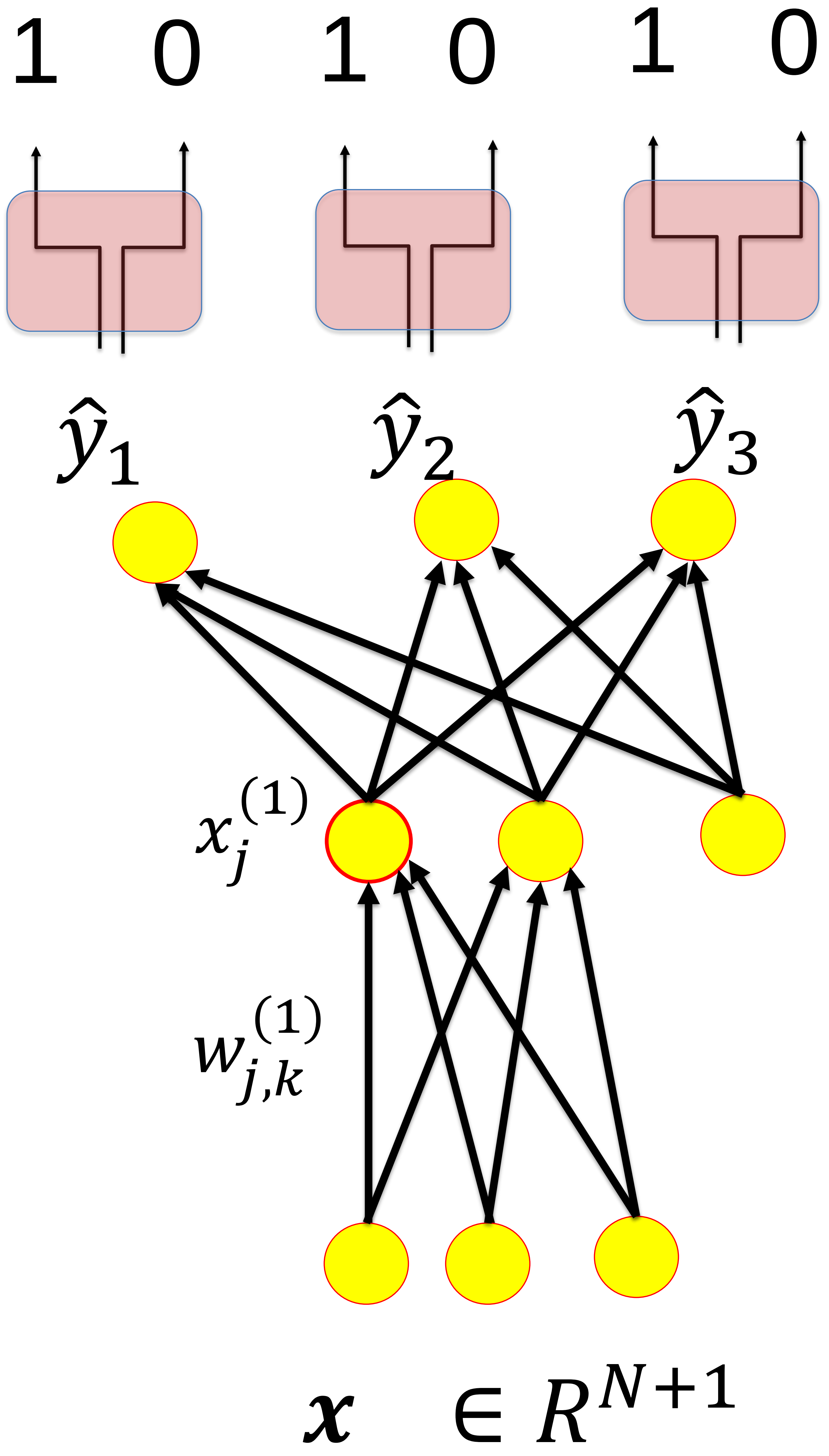


5. Softmax output

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

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





Artificial Neural Networks: Lecture 3

Statistical Classification by Deep Networks

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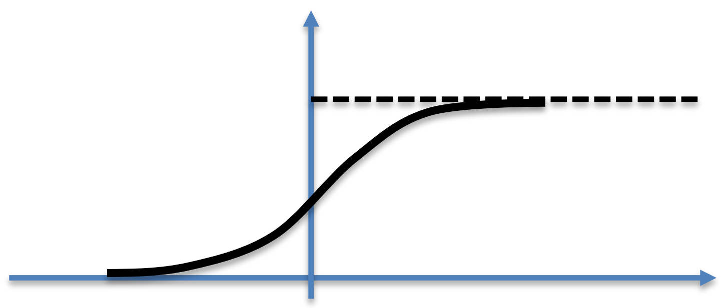
1. The statistical view: generative model
2. The likelihood of data under a model
3. Application to artificial neural networks
4. Multi-class problems
5. Sigmoidal as a natural output function
6. **Rectified linear for hidden units**

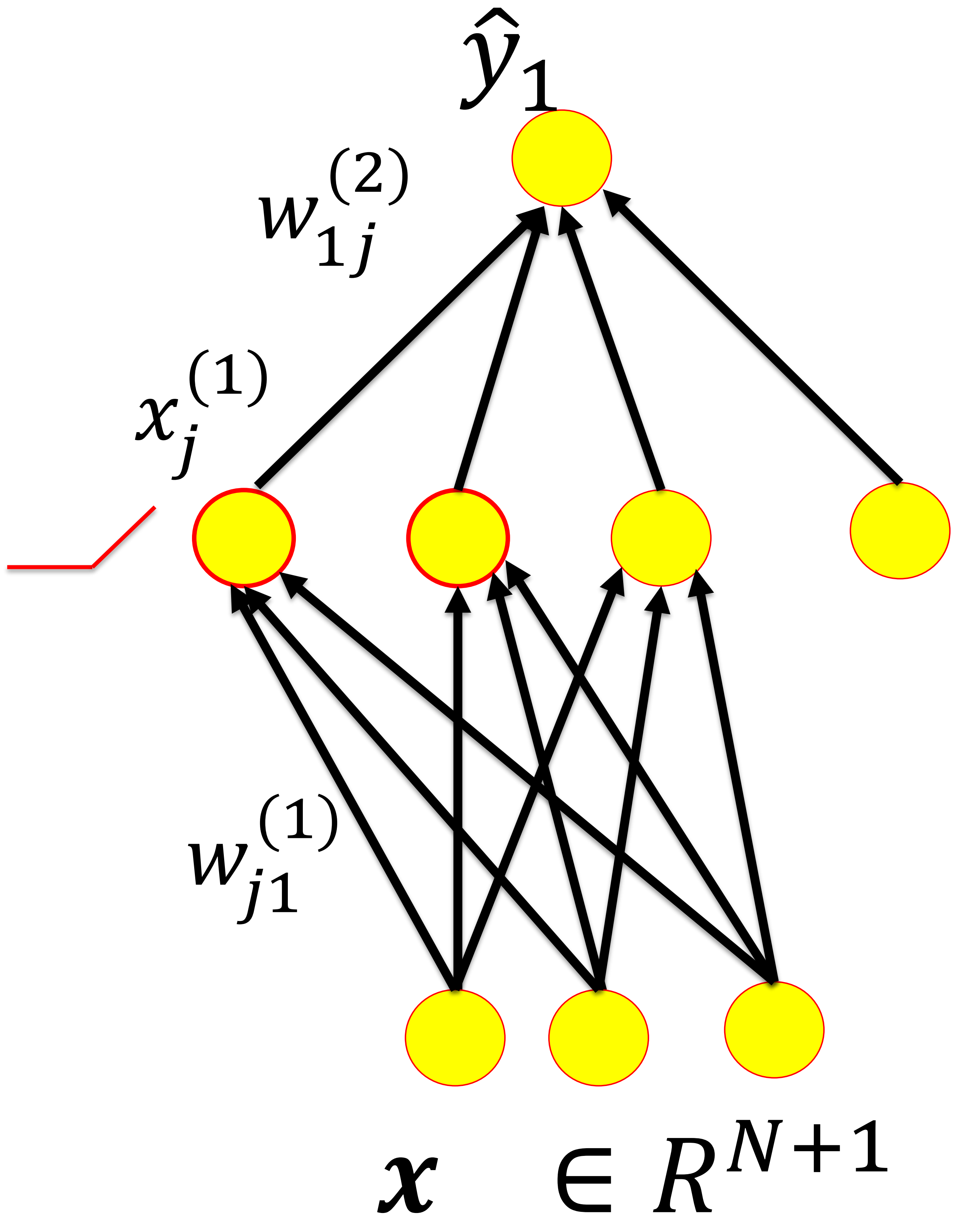
6. Modern Neural Networks



output layer

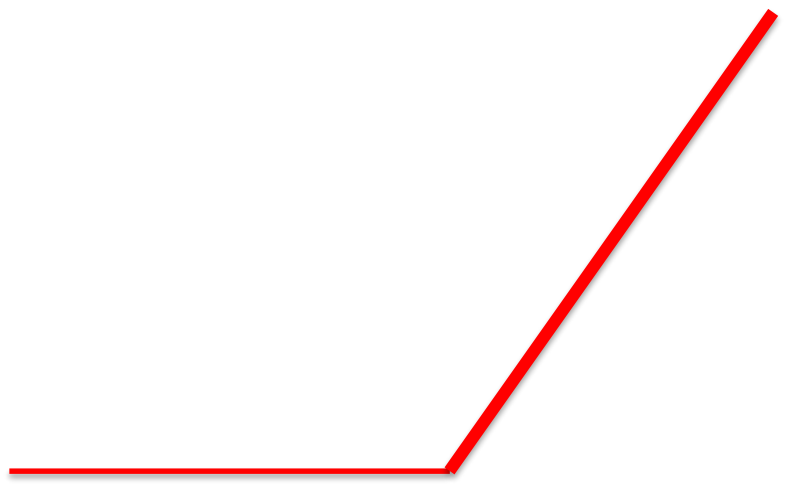
use sigmoidal unit (single-class)

or softmax (exclusive mutlit-class)



hidden layer

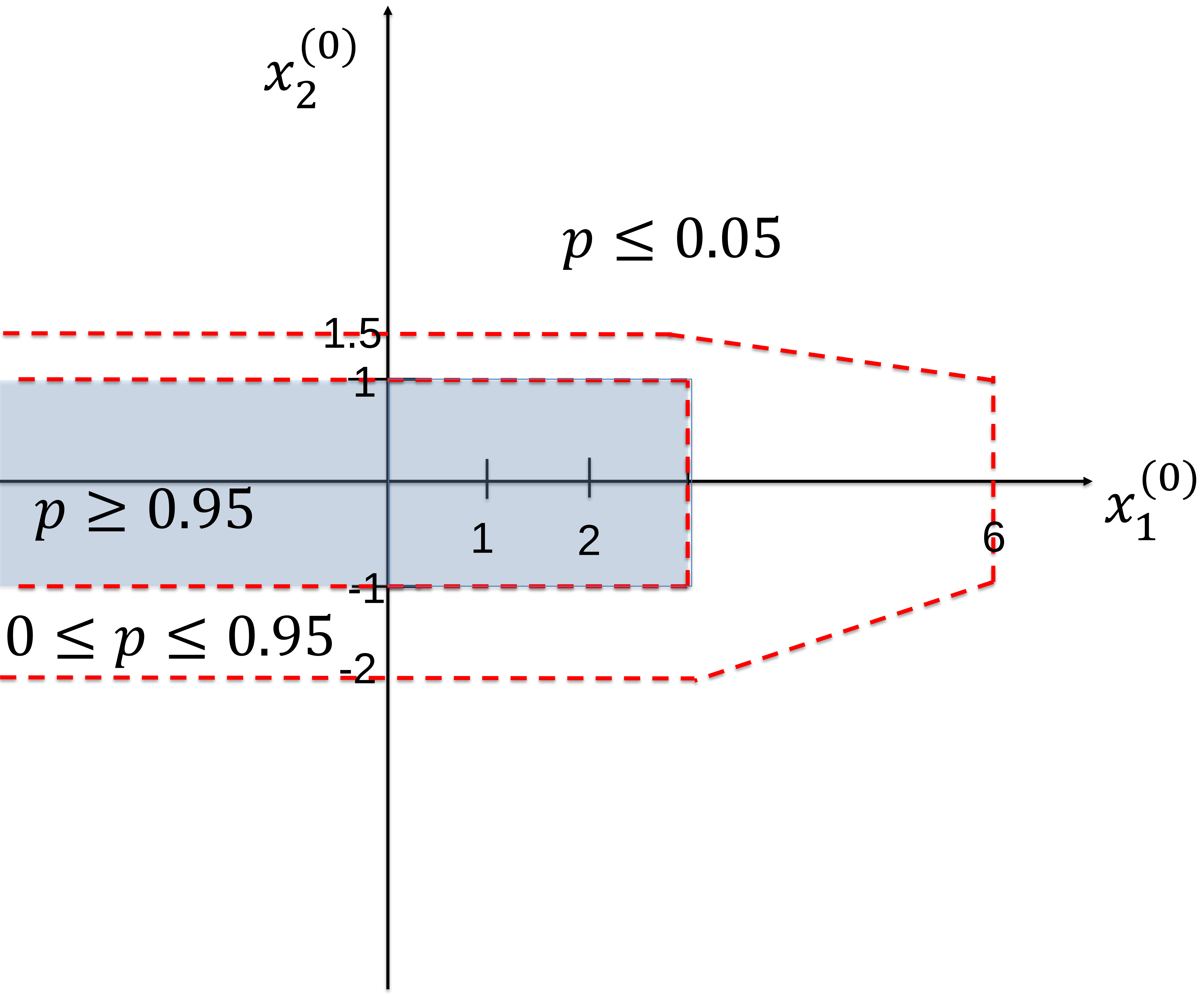
use rectified linear unit in $N+1$ dim.

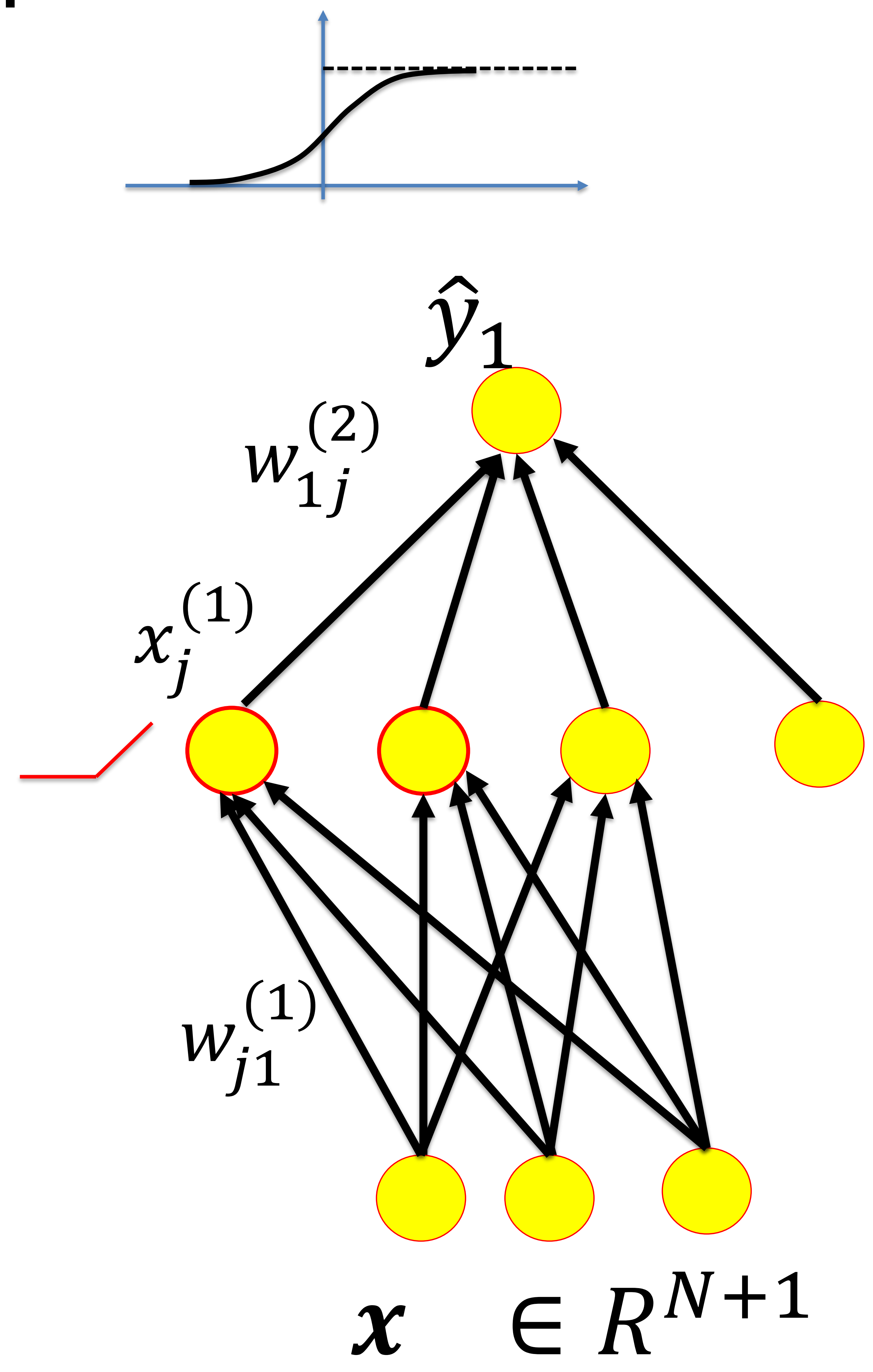


$f(x)=x$ for $x>0$

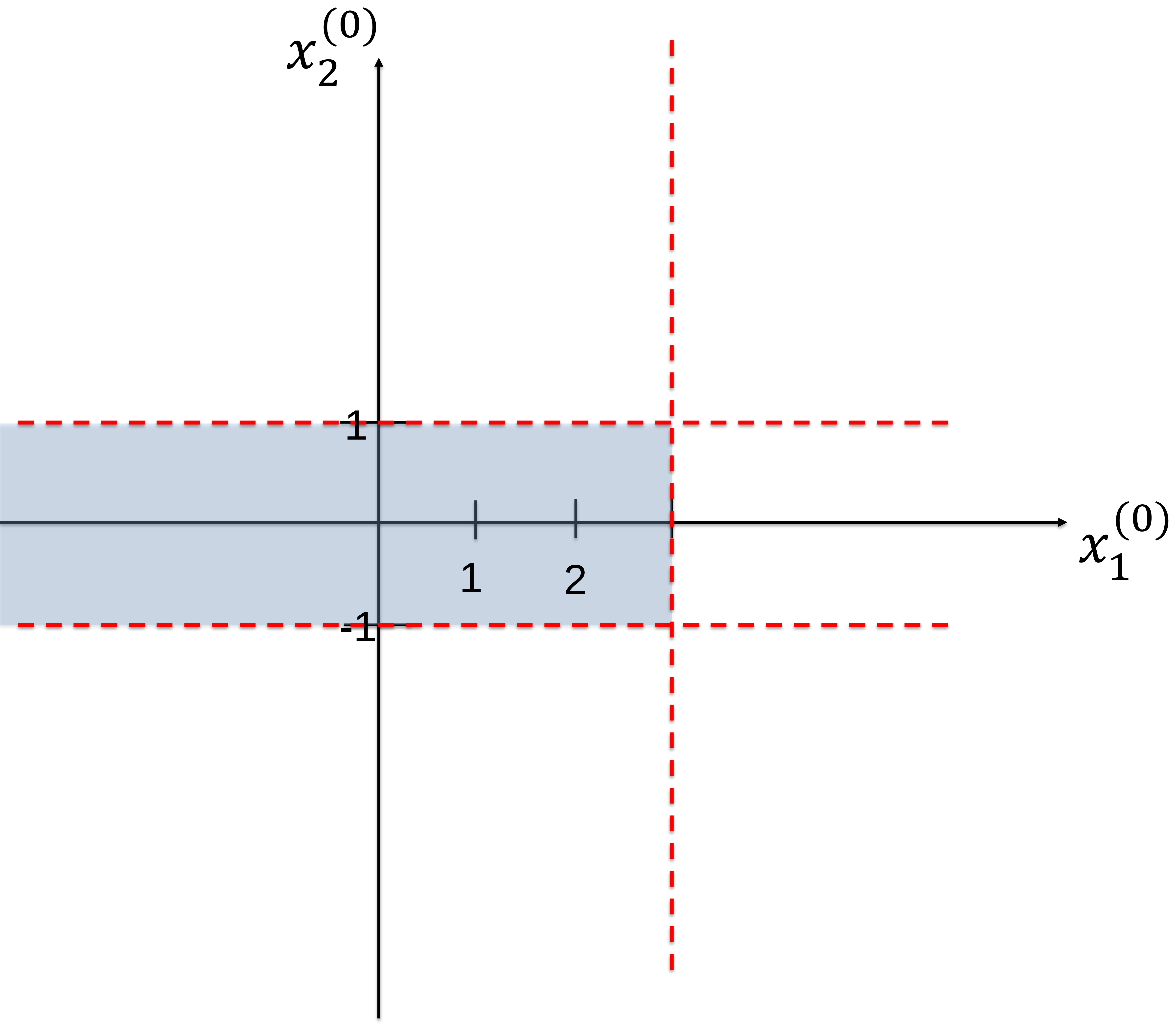
$f(x)=0$ for $x<0$ or $x=0$

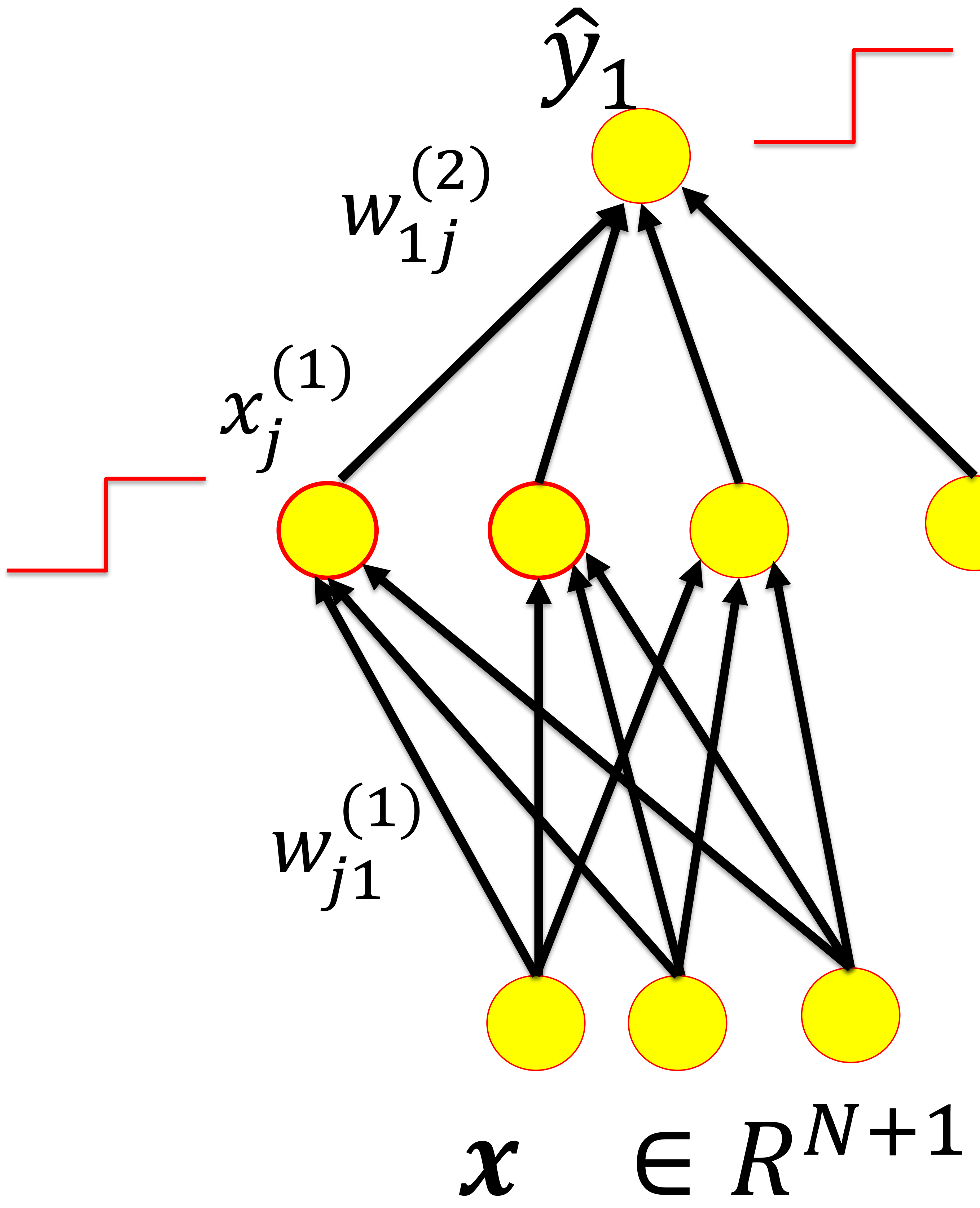
Preparation for Exercises:
Link multilayer networks to probabilities





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 with 1-hot coding
[ ] sigmoidal unit should be used for single-class problems
[ ] two-class problems are the same as single-class problems
[ ] multiple-attribute-class probalems are the same a single-class
[ ] it’s great we can interpret the output as a probability, because

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

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

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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 by ‘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 and 3.13 of

Deep Learning