Ch4. Artificial Neural Networks 4.1 - 4.7

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Biological neural systems

- Each neuron has
  - Soma = cell body
  - Dendrites = multiple inputs
  - Axon = output

- Synapse
  - Connects an axon to a dendrite
  - Might increase (excite) or decrease (inhibit) a signal
  - When input signal sufficiently strong → neuron fires (= propagates signal)

- No. of neurons in human brain ~ 10^{10}

- Connections per neuron ~ 10^{4}

- Face recognition ~ 0.1 sec

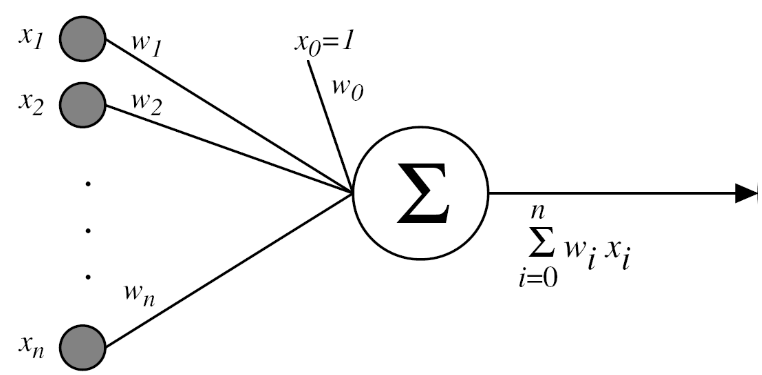
- Neuron switching time ~10^{-3} sec

- Highly parallel & distributed processing

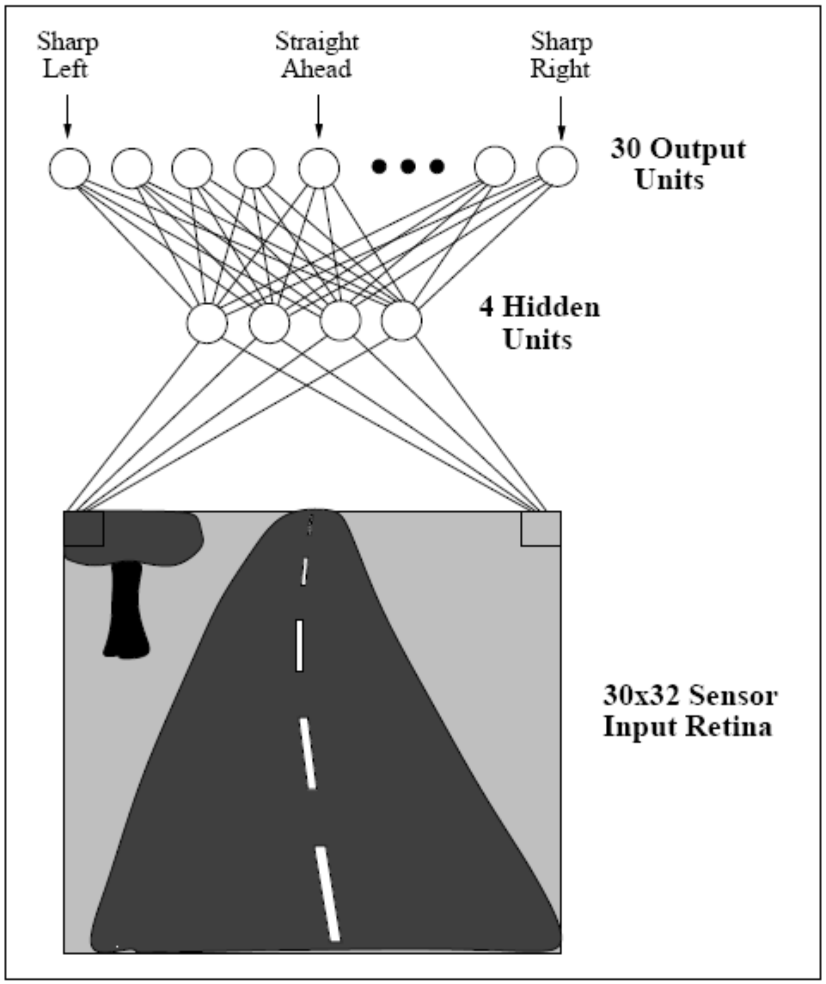
Artificial neural networks (ANN)

- Consist of
  - Units
  - Connections
  - Weights
- Learn to associate inputs to outputs by tuning the weights
- E.g.
  - Input = pixels of photo
  - Output = classification of photo (landscape?, car?,…)
- Highly parallel & distributed processing

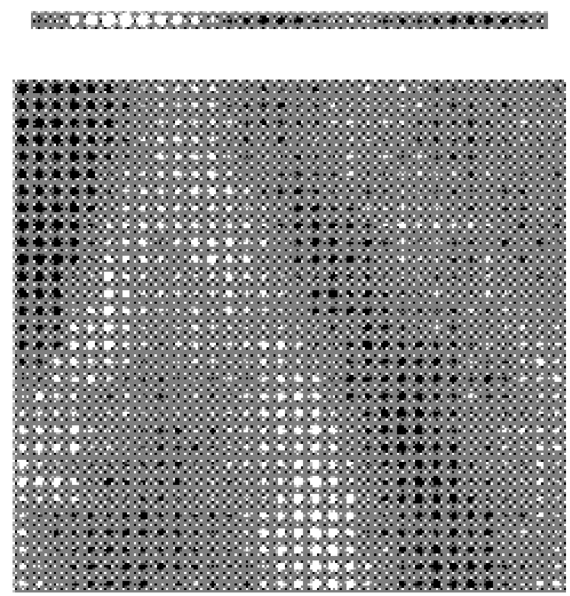
Biological NN	**Artificial NN**
Soma	Unit
Axon, dendrite	Connection
Synapses	Weights
Threshold	Bias
Signal	Activation function



Ex. – ALVINN [Pomerleau 1989] drives 70mph on highway



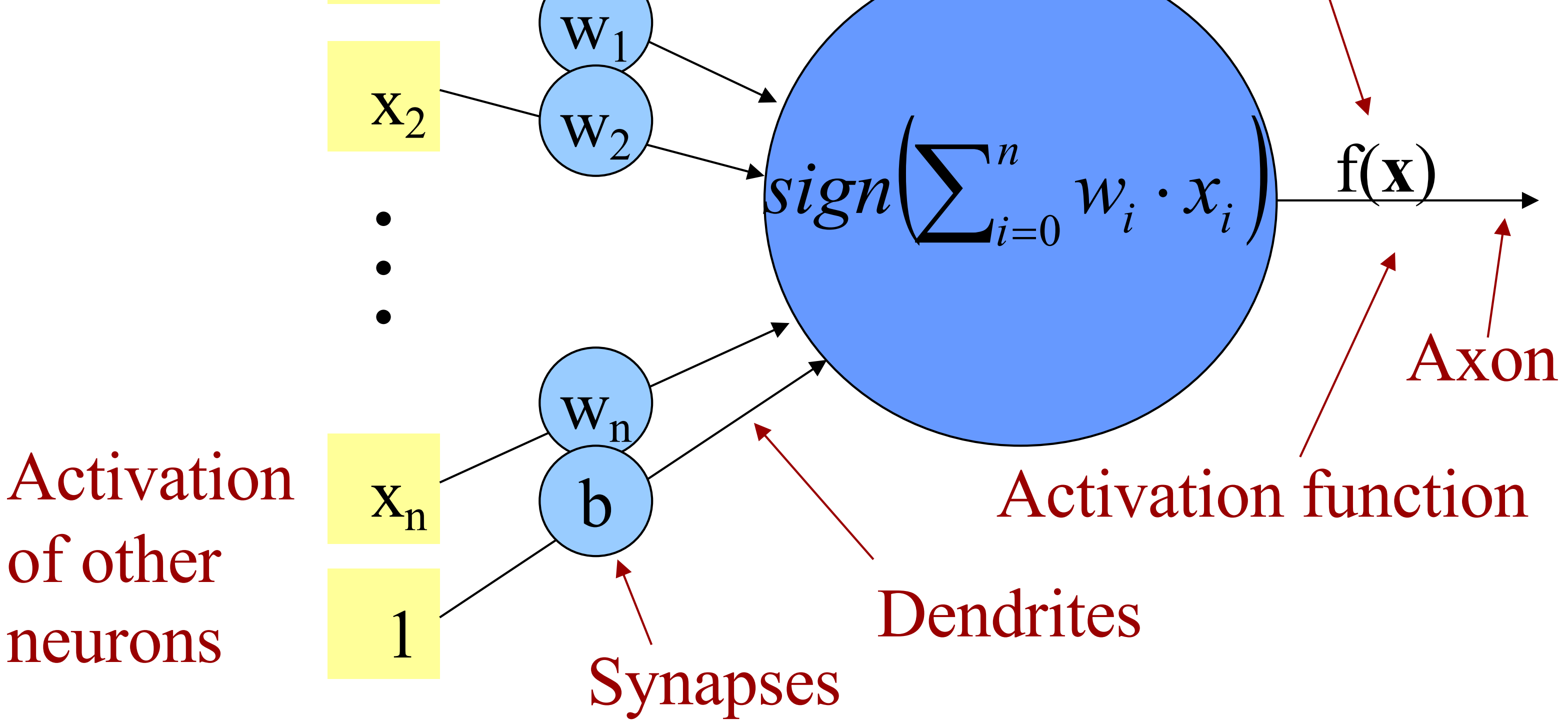
Autonomous Land Vehicle in a Neural Net



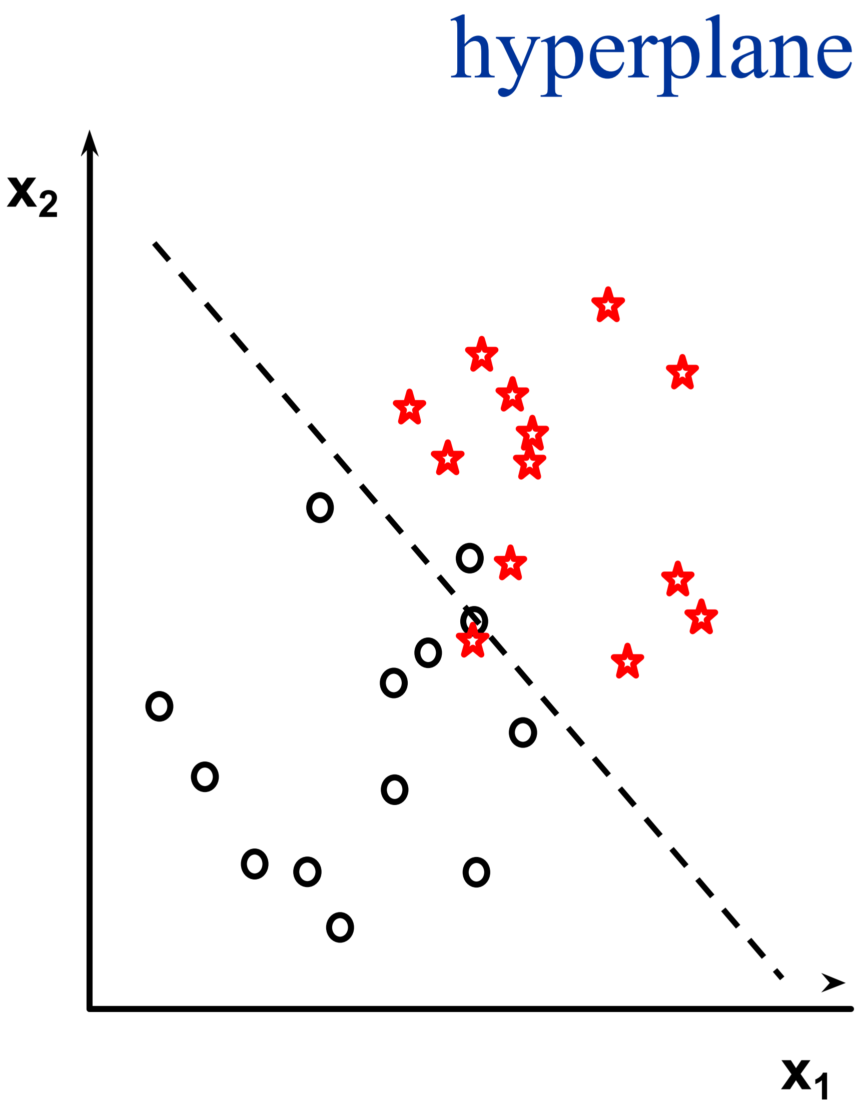
Perceptron

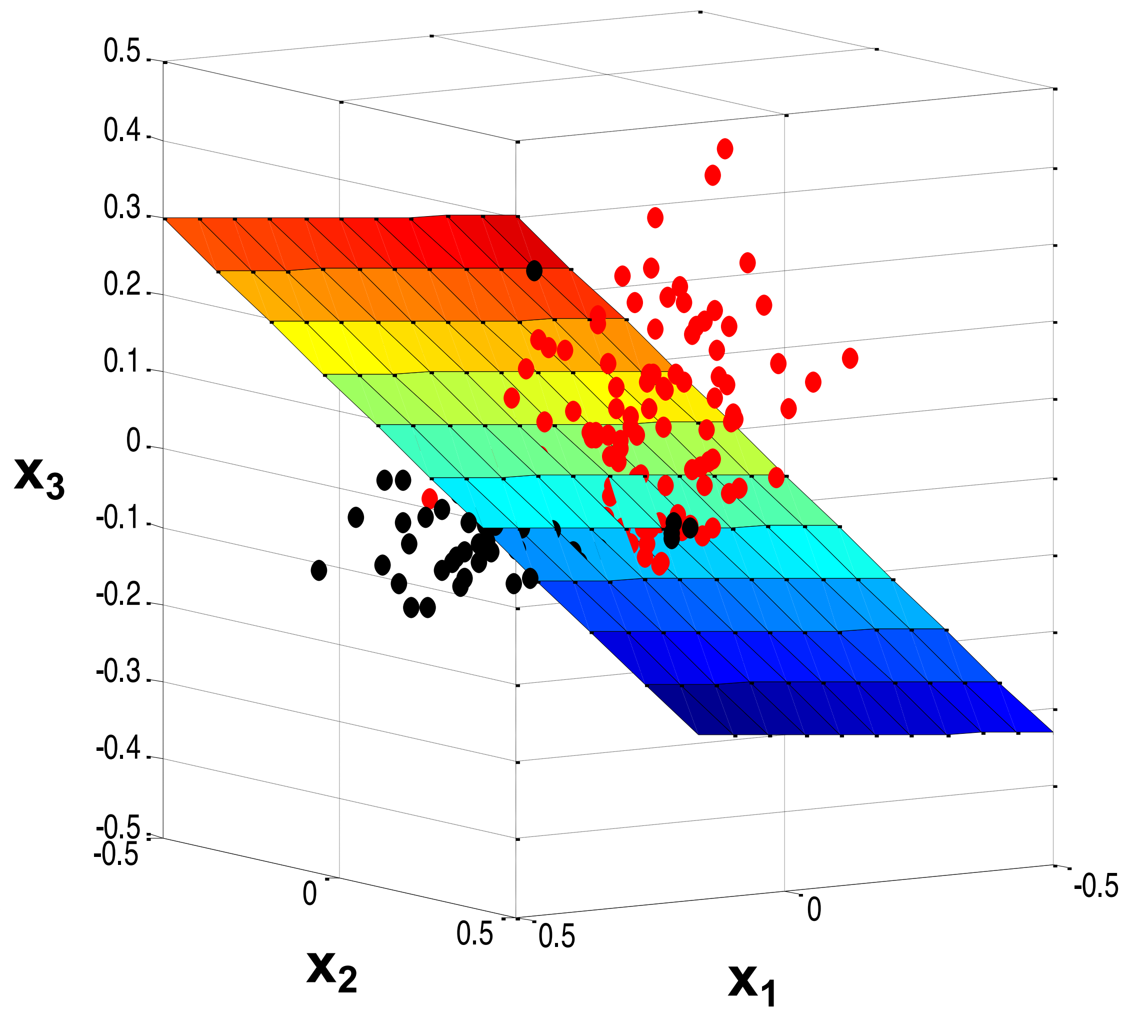
- Simplest NN → simulates 1 neuron
- o(x)=sign$\left(\sum_{i=0}^{n} w_i \cdot x_i\right)$

$$o(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \cdot \vec{x} > 0 \\ -1 & \text{otherwise.} \end{cases}$$

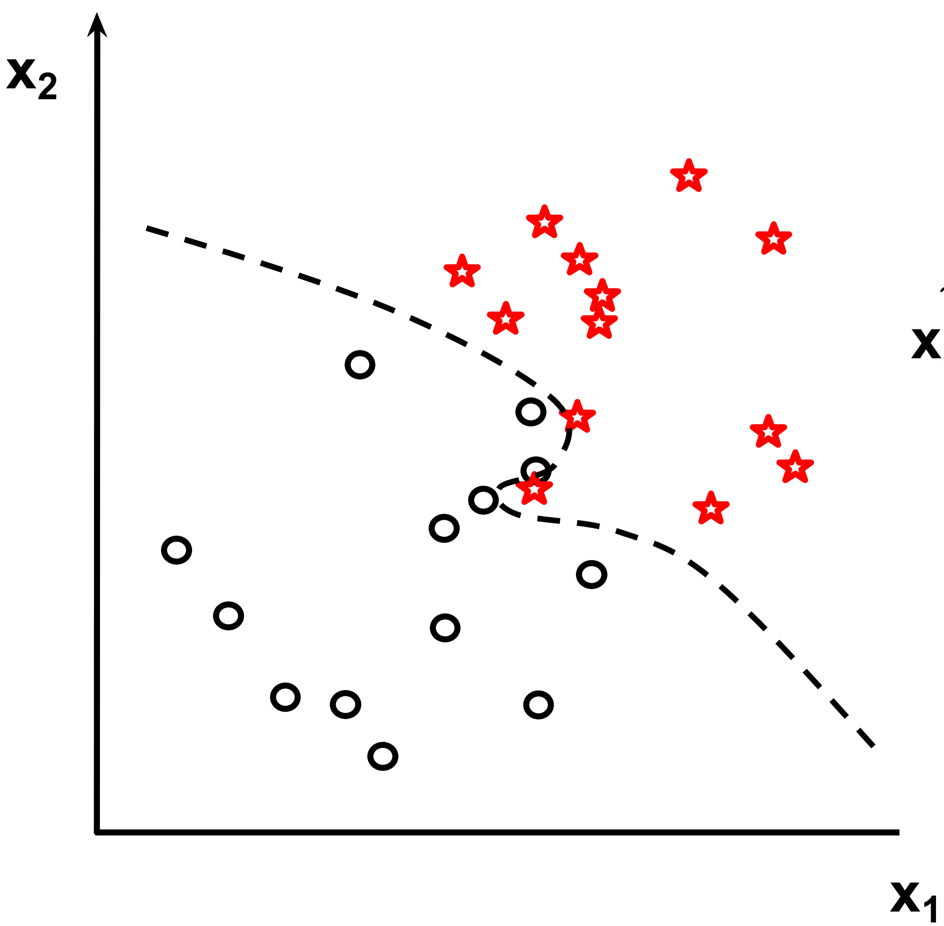


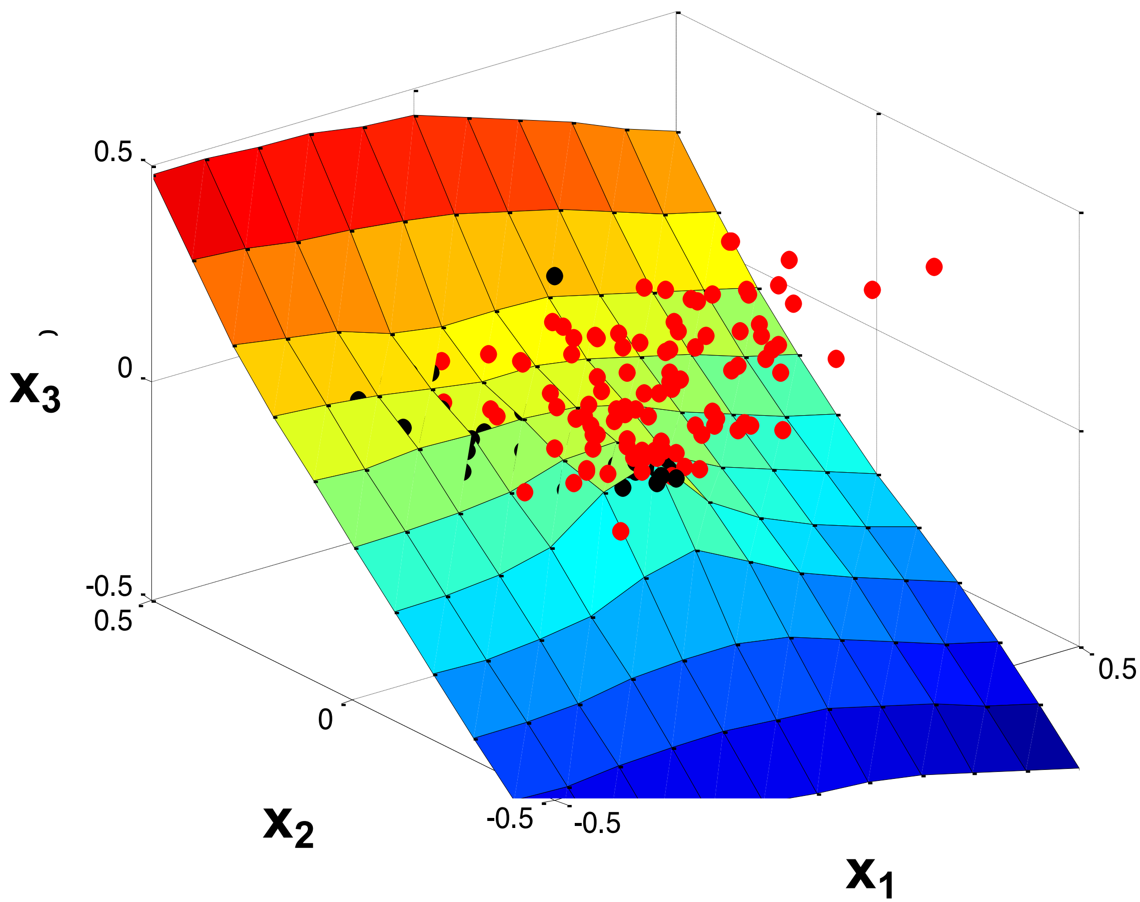
Linear decision boundary





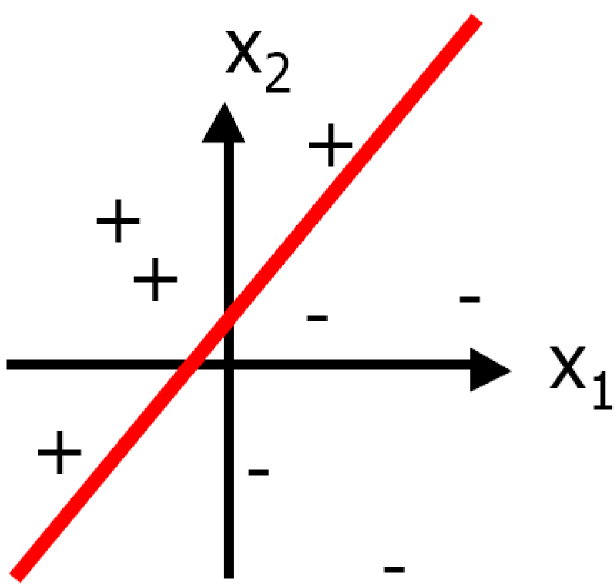
Non-linear decision boundary

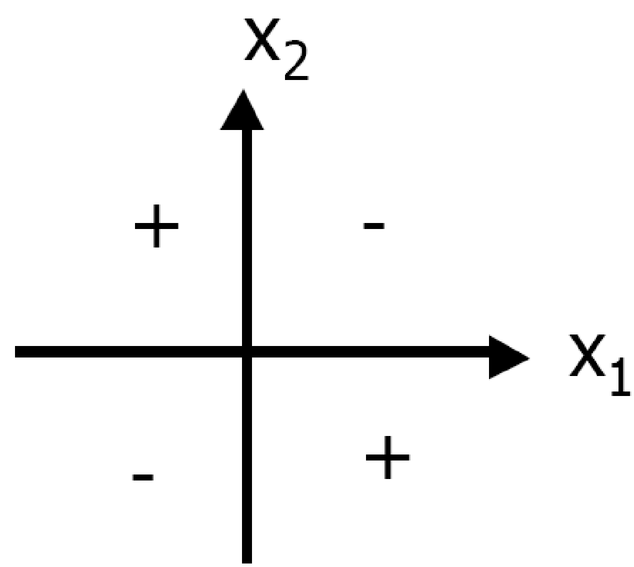




Perceptron – decision surface

- Hyperplane ("line") in an n-dimensional space
- Find a Perceptron to solve the AND pb. for two inputs x_1, x_2 → w_i=?
- Functions not linearly separable (e.g. XOR) → not representable with only one neuron ➔ use more neurons ➔ neural network (NN)





Perceptron – learning rule

$$w_i \leftarrow w_i + \Delta w_i$$

where

$$\Delta w_i = \eta(t - o)x_i$$

Where:

- $t = c(\vec{x})$ is target value
- o is perceptron output
- η is small constant (e.g., .1) called *learning rate*

- If o correct (t = o)➔ weights w_i are not changed
- If o incorrect (t = o)➔ weights w_i are changed s.t o is closer to t
- Algorithm converges to correct classification if
  - Training data is linearly separable
  - Learning rate is sufficiently small

Gradient descent – learning rule

- Consider perceptron without threshold (i.e. no sign(o)) and continuous outputs o (not just 1, -1)

- Train w_i s.t. they min the squared err (LMS-least mean squared error)

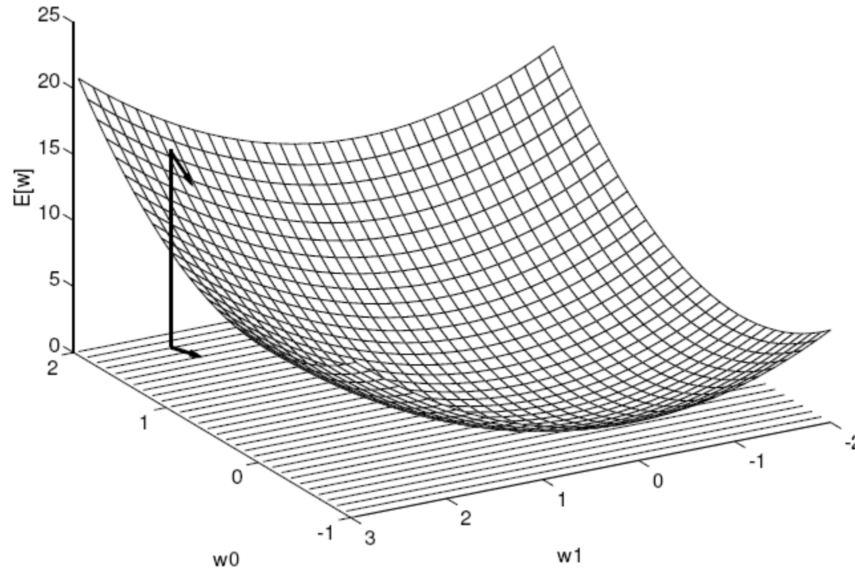
$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

where D is the set of training data

Gradient descent

- = steepest descent rule = delta rule = LMS rule = Widrow-Hoff rule
- Name "delta rule" (Widrow-Hoff rule) comes from

$$\Delta w_i = \eta(t - o)x_i$$



- Finds local minima by taking steps opposite to the gradient
- Gradient = vector with the greatest rate of increase
- Small learning rate → algorithm converges

Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right]$$

Training rule:

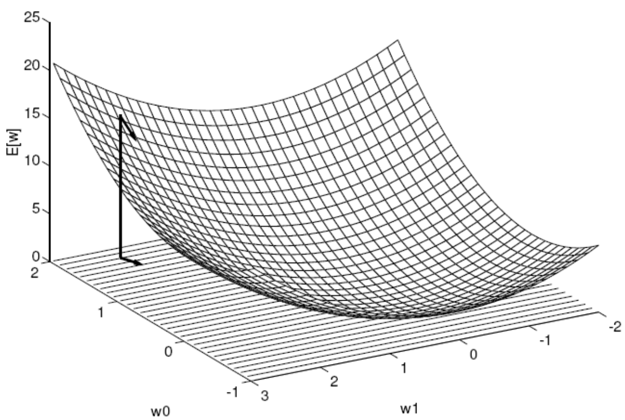
$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

Gradient descent

$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$



Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right]$$

Training rule:

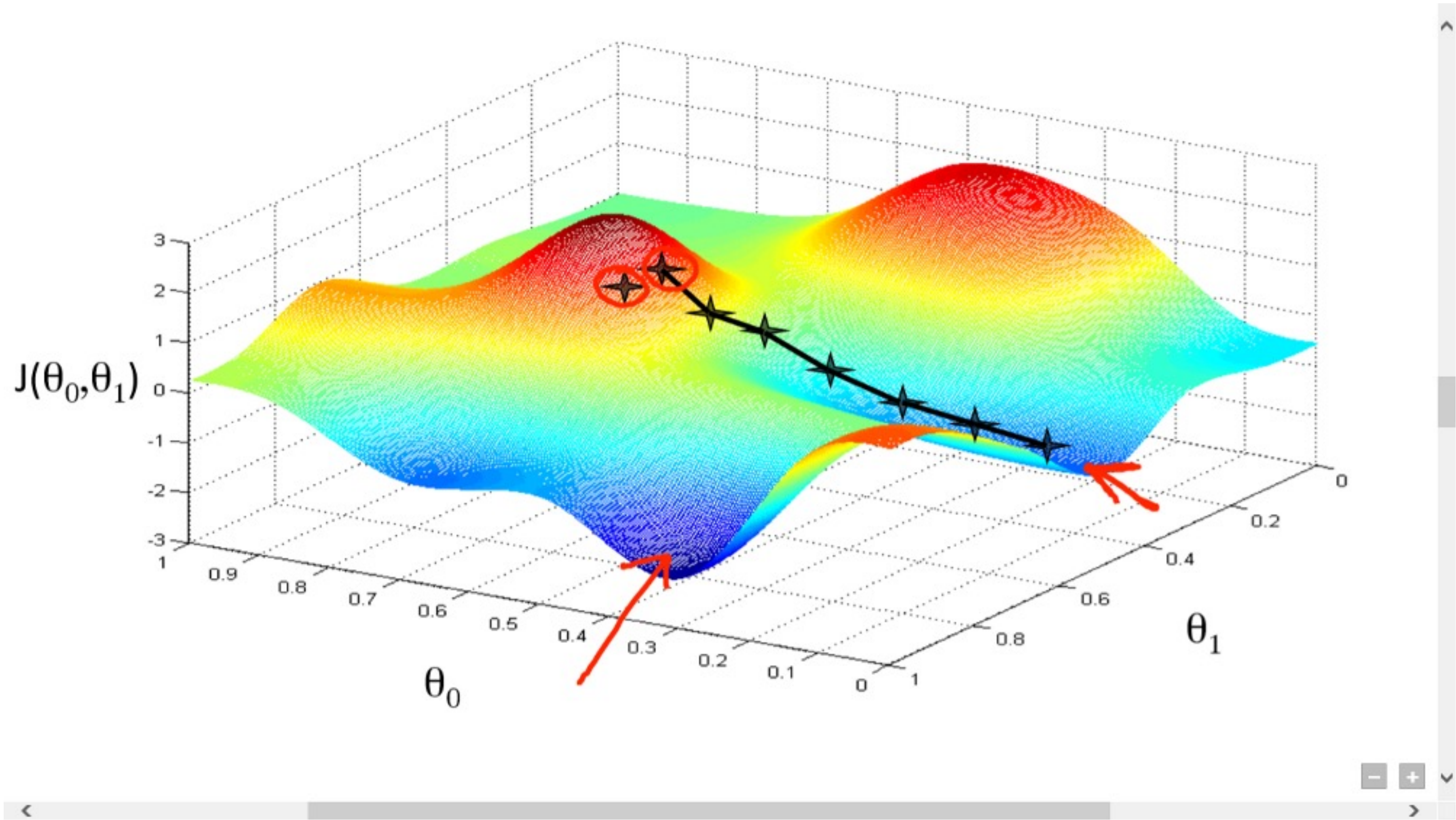
$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

$$\begin{aligned} \frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\ &= \sum_d (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{w} \cdot \vec{x_d}) \\ \frac{\partial E}{\partial w_i} &= \sum_d (t_d - o_d)(-x_{i,d}) \end{aligned}$$

Gradient descent illustration



You might miss the global minima on error surface.

Perceptron algorithm

- Ip: tr. ex., η
  - Each tr. ex is a pair <$(x_1,\ldots, x_n)$, t>
- Op: w

1. w init. with small random values
2. Until termination cond. met do
   1. each $\Delta w_i = 0$
   2. For each tr. ex. <$(x_1,\ldots, x_n)$, t> do
      1. Input the instance $(x_1,\ldots, x_n)$ to the neuron and compute o
      2. For each w_i do

         $\Delta w_i = \Delta w_i + \eta(t-o)x_i$ %accumulates change from each tr.ex
   3. For each w_i do % o(sign(w*x)), uses sign fct

      $w_i = w_i + \Delta w_i$ %update w only once → batch mode

Gradient descent

Batch mode Gradient Descent:
Do until satisfied

1. Compute the gradient $\nabla E_D[\vec{w}]$
2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$

Incremental mode Gradient Descent:
Do until satisfied

- For each training example d in D
  1. Compute the gradient $\nabla E_d[\vec{w}]$
  2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$

Gradient descent - conclusions

- Finds a solution that minimizes the error
  - ➔ works also for non-linearly separable data (unlike perceptron!)
  - ➔ tolerates noisy data

- Local minima (= minimum error) obt. by taking steps opposite to the gradient

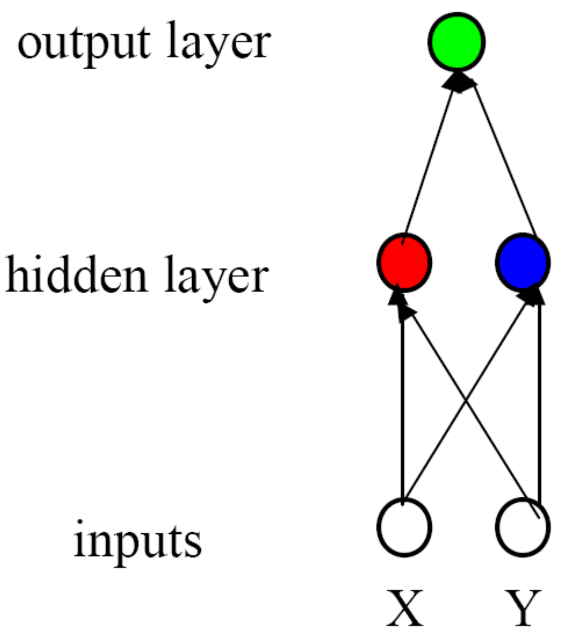
- Small learning rate → algorithm converges

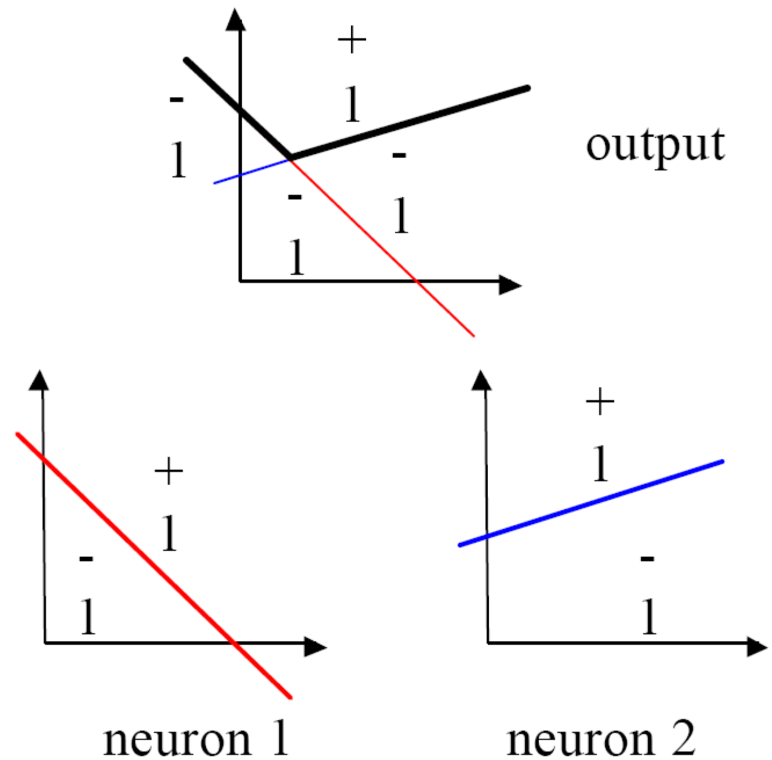
- Weaknesses
  - Slow convergence
  - If not small enough learning rate → might miss the min

- Limitations for both perceptron and gradient descent
  - Solve only a small class of pb.
  - → Combine many neurons in a network

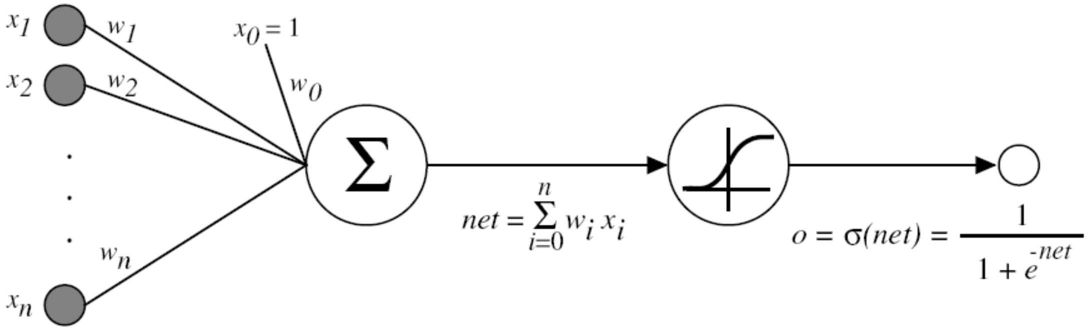
Multilayer networks

- Increase representation power





Sigmoid unit



$\sigma(x)$ is the sigmoid function

$$\frac{1}{1+e^{-x}}$$

Nice property: $\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$

We can derive gradient decent rules to train

- One sigmoid unit
- *Multilayer networks* of sigmoid units $\rightarrow$ Backpropagation

- Graph σ

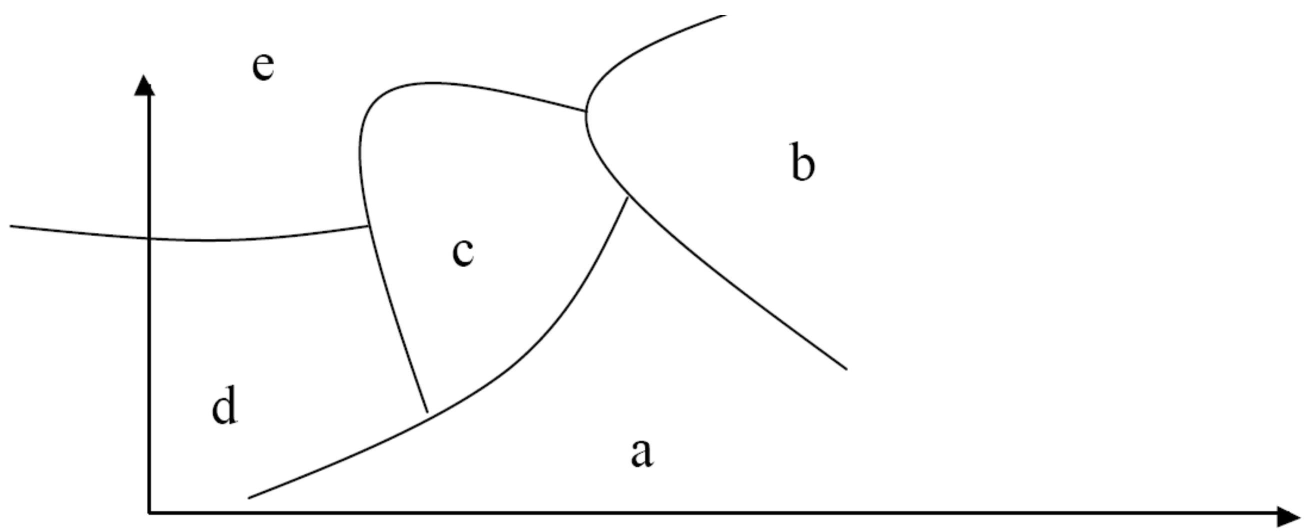
```
x=(-10:0.1:10);
y=1./(1+(2.71).^(-x));
plot(x,y);
```

- Can you understand why is called squashing function?

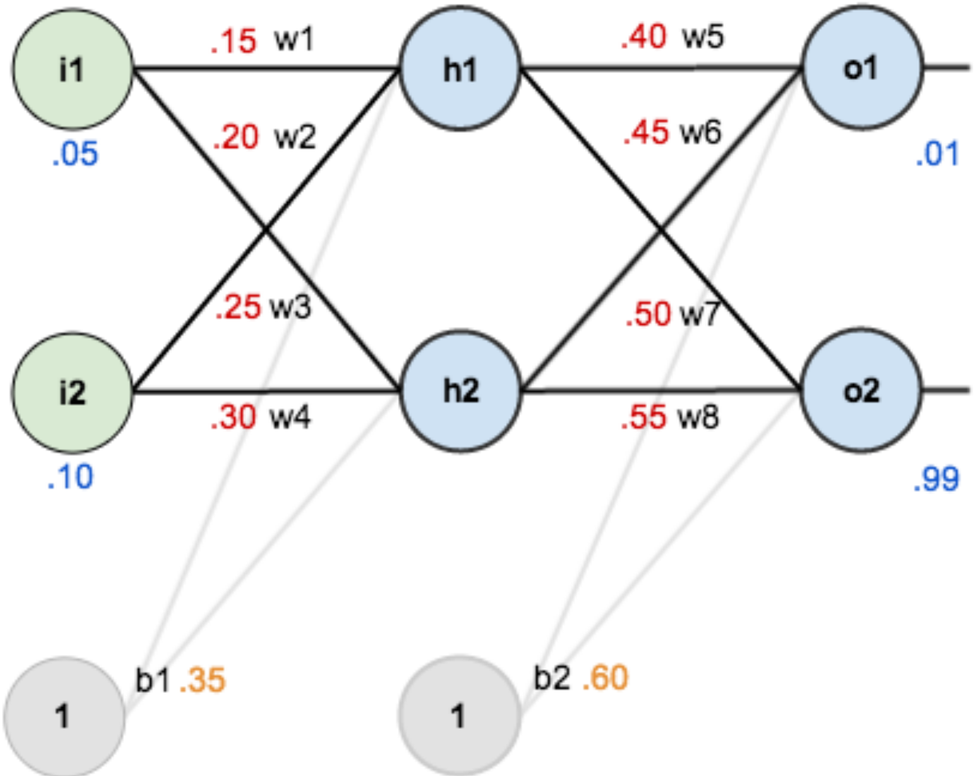
- aka. logistic function

Sigmoid unit

- Causes non-linear decision surface
- Very powerful representation
- OBS. Multiple layers of linear units still produce only linear functions ➔ use non-linear activation fct.



Examples of NN and 1-to-N encoding



5) Ex. of 1-to-N
Data with Class label =
[data1 2
 data2 3
 data3 1
 data4 3
 …]

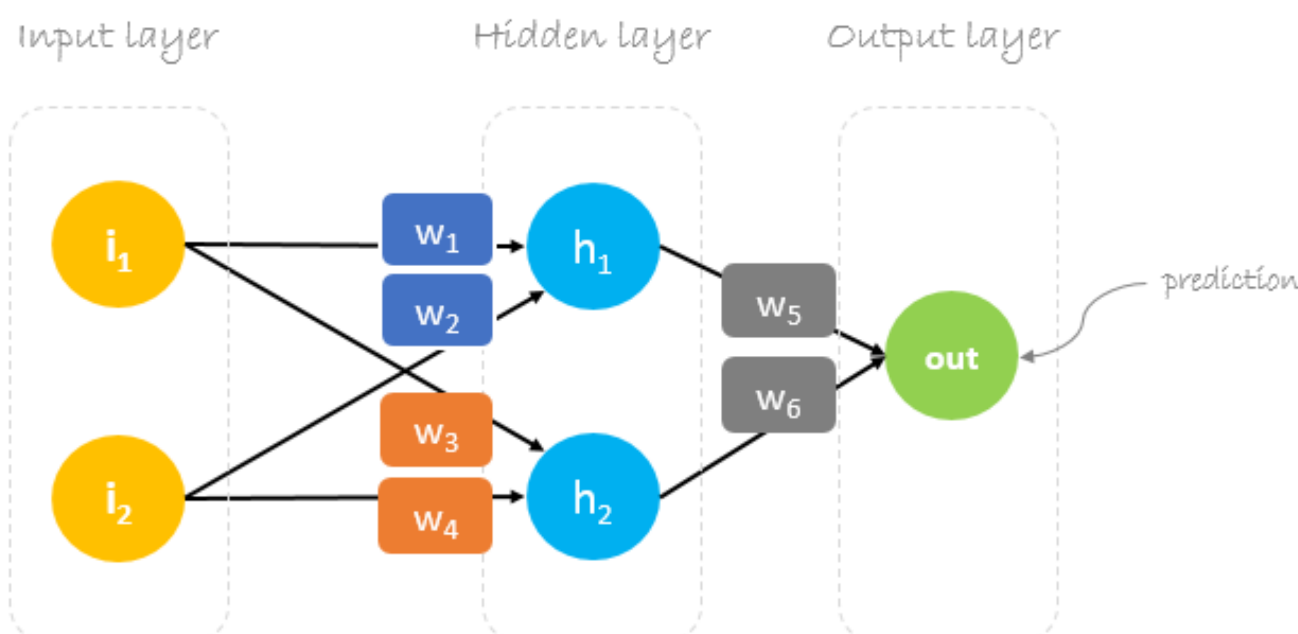
Class label encoded =
[0 1 0
 0 0 1
 1 0 0
 0 0 1
 …]

1) If using sigmoid activation fct. ➔ output in [0,1]

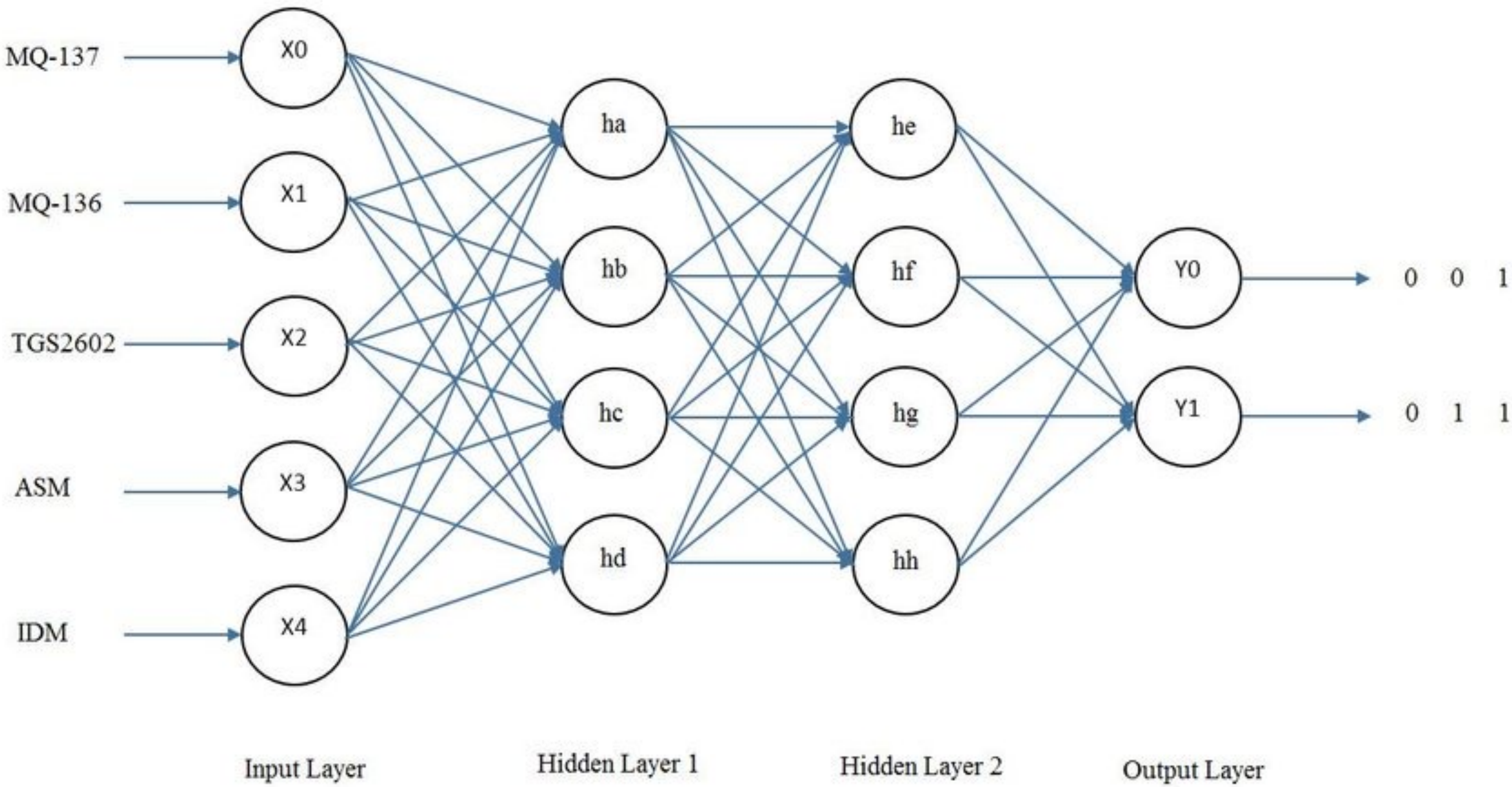
2) What is the difference between using 1 vs 2 output neurons?
Assume, a 2-class classification problem.
It is easier to learn outputs
[1 0] as class 1
[0 1] as class 2

3) For 3-class classification this is even more obvious:
[1 0 0] is output for class 1, etc.

4) Explain what happens in neuron h2?
What is the input? What is the output?
Write the math/answer on your notebook.

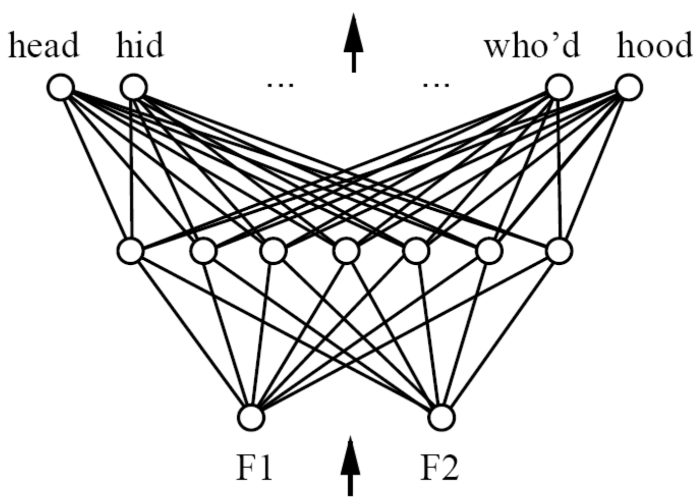


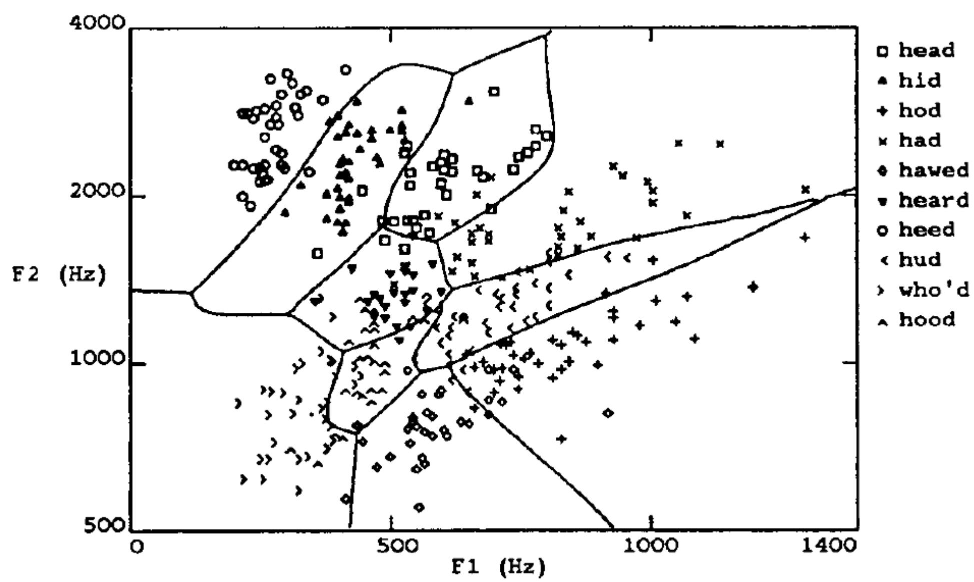
Examples of NN



Multilayer NN with sigmoid units

- Speech recognition
- Data from spectral analysis of the sound
- 10 outputs





Backpropagation algorithm

Initialize all weights to small random numbers.
Until satisfied, Do

- For each training example, Do
  1. Input the training example to the network and compute the network outputs
  2. For each output unit k

$$\delta_k \leftarrow o_k(1-o_k)(t_k-o_k)$$

  3. For each hidden unit h

$$\delta_h \leftarrow o_h(1-o_h) \sum_{k \in outputs} w_{h,k}\delta_k$$

  4. Update each network weight $w_{i,j}$

$$w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}$$

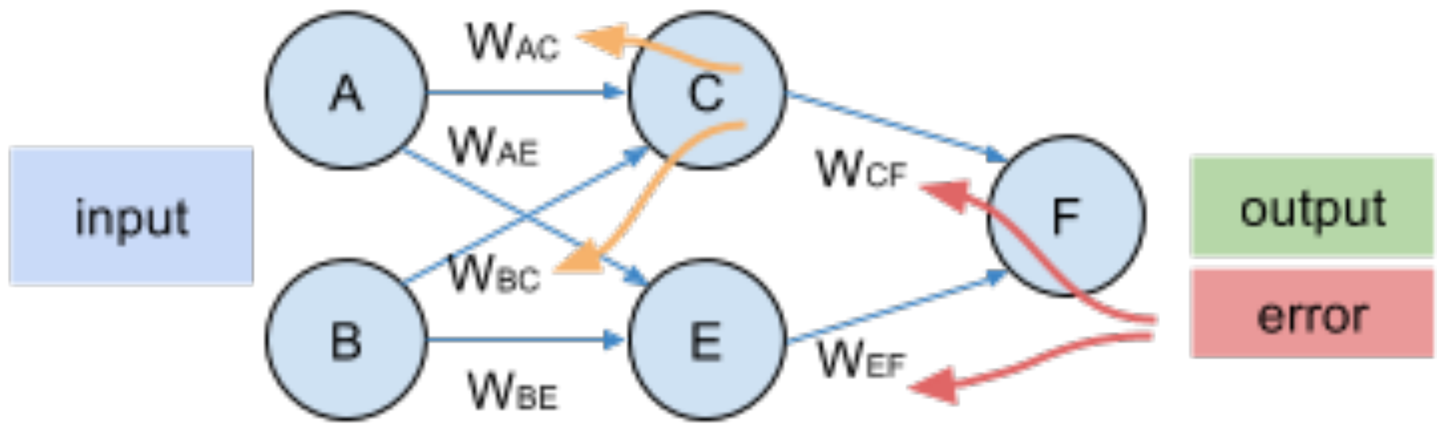
where

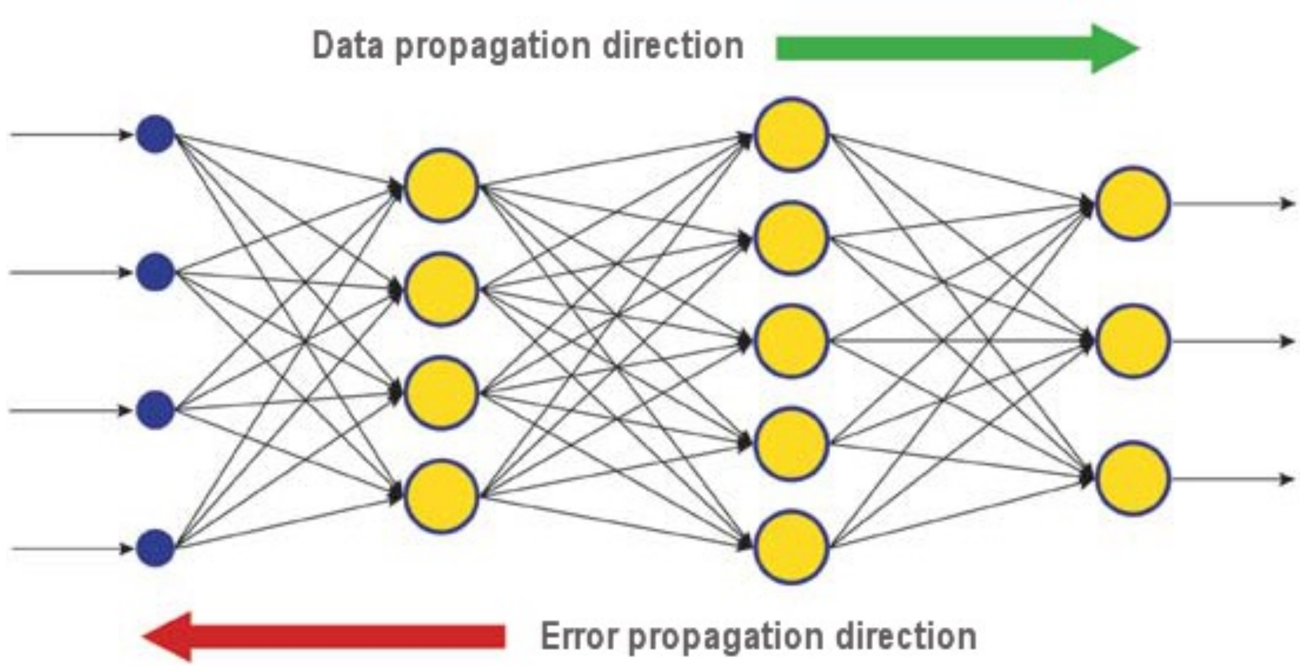
$$\Delta w_{i,j} = \eta \delta_j x_{i,j}$$

Obs. 1 Steps 2, 3 and 4 propagate the err backward through NN

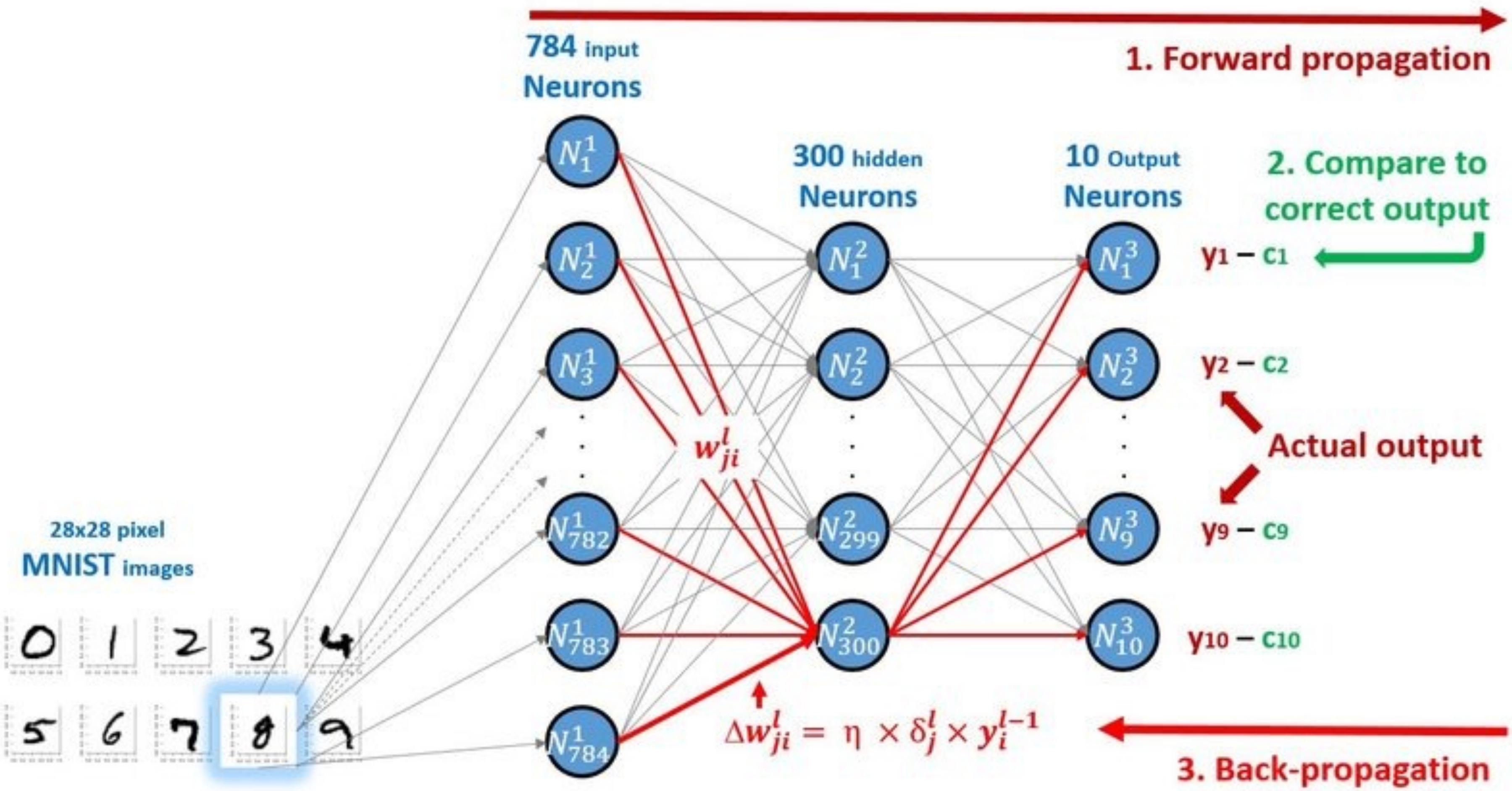
Obs. 2 Initial w near zero → init. net near-linear (see logistic fct. around 0) → increasingly non-linear functions possible as training progresses

Backpropagation illustration

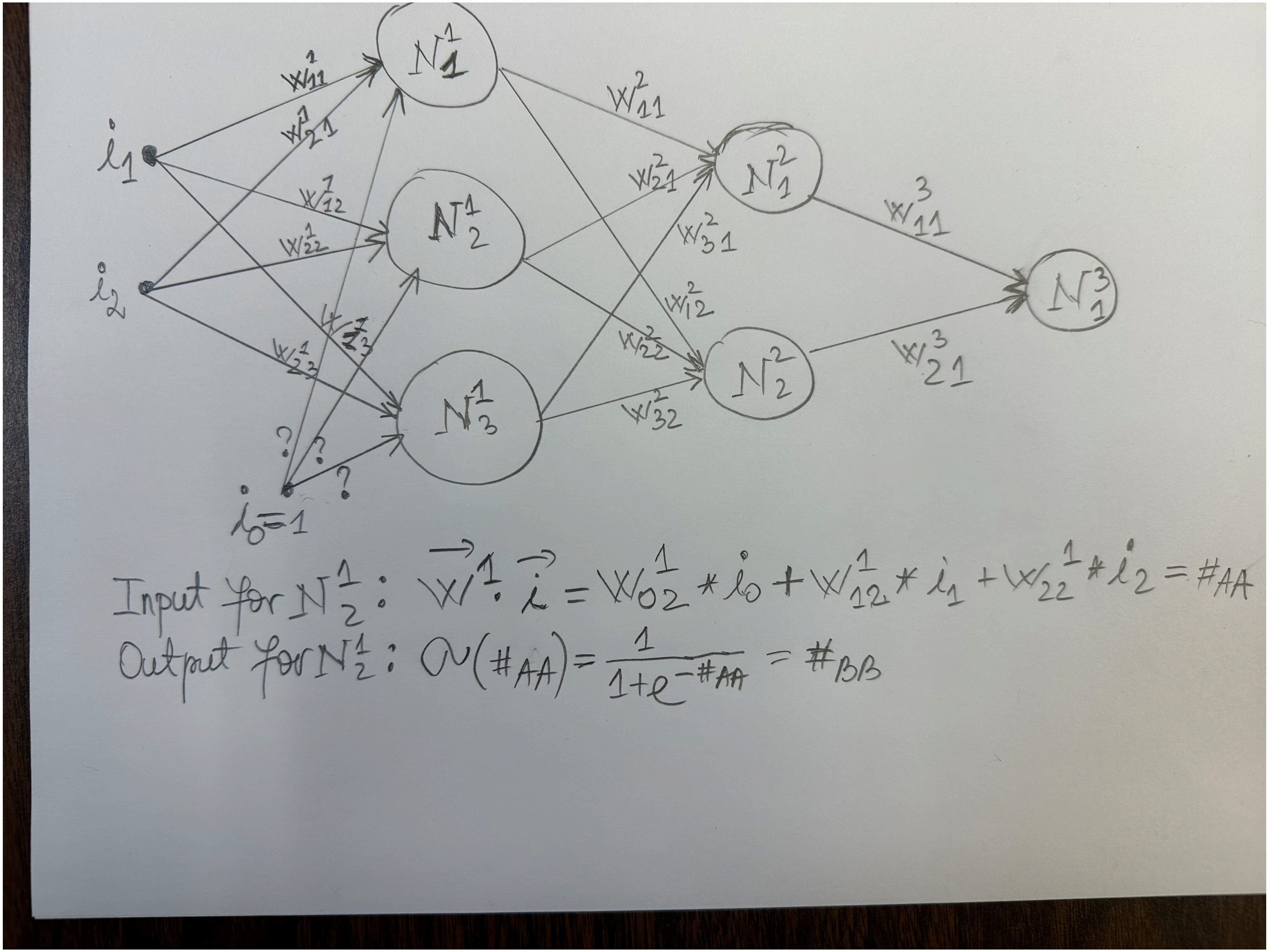




NN for classifying hand-written digits



NN notations



Bias in Backpropagation FNN

- Mitchel: interpolates two pos. ex. that do not have a intervening negative, with a pos.

- Net topology chosen by trainer
  - # of layers
  - # of neurons
  - transfer fct.
  1. many hidden layers and neurons
     - → powerful net
     - → can approx. many hypotheses
     - → weak inductive bias → poor generalization
  2. smaller hidden layers and neurons
     - → weak net
     - → can approx. fewer hypotheses
     - → stronger inductive bias
     - → PREFFERED: an h that approx. well t from training has higher probability of well approx. the actual (TRUE) t

- GOAL: find the weakest topology to learn the training data → strongest inductive bias → best generalization

Overfitting in Backpropagation FNN

- “memorize” training data, but cannot generalize

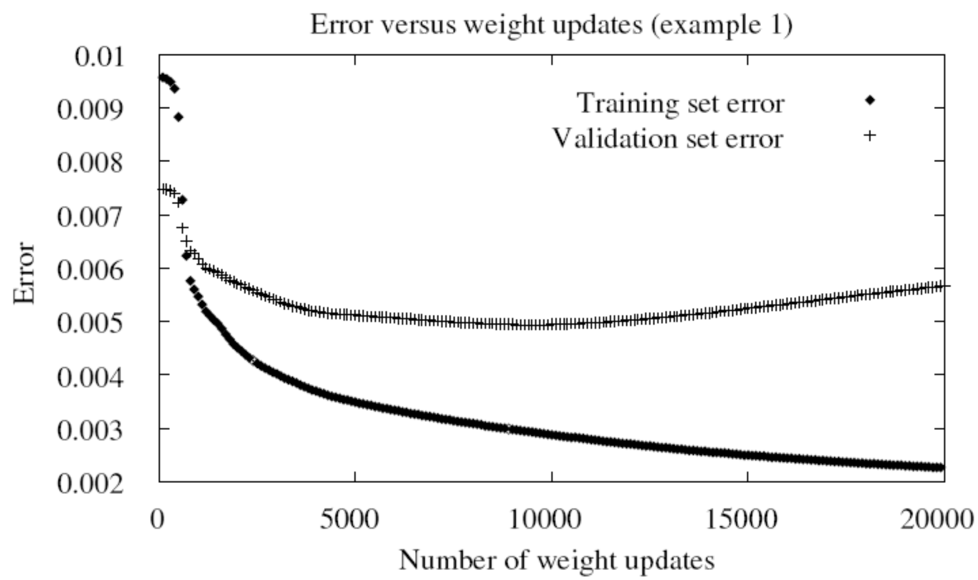
- Choice of too powerful a net provides with excessive # of h, thus making available h that fit tr. data but do not match t well

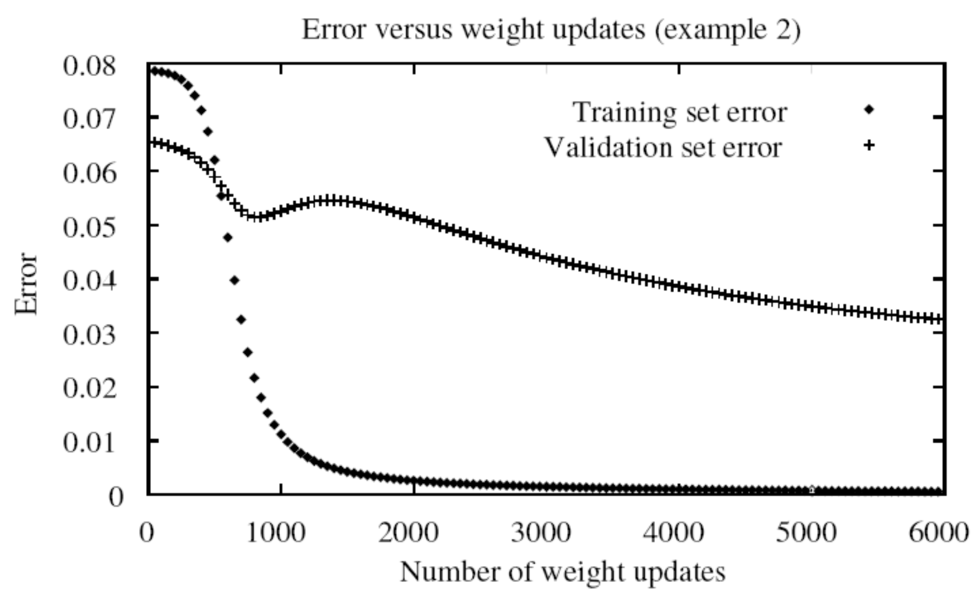
- May use a powerful net + add some bias
  - weight-decay
    - adds bias by decreasing all w by a small amount at each iteration → non-reinforced weights get smaller
  - k-cross validation
    - split tr. data in k subsets, train k different nets by using one of the k parts for test and remaining k-1 for training → select the net that generalizes best

- OBS. More than 1 or 2 layers on neurons leads to overfitting

More about overfitting

- Tr. data is not representative of general distribution of examples
- After many iterations, Backpropagation will create overly complex dec. surface that fits noise
- Solution:
  - Use validation set
  - k-cross validation (if little data)
- One can discover the best net at unpredictable time (keep a running w of min err), e.g. top figure shows best net at epoch~9000





Backpropagation algorithm

- Gradient descent over entire network weight vector
- Min error over training ex.
- Finds local (not always global) min – err surface has multiple local min!!
- However, in practice works well – run it multiple times with different random initial weights
- Slow training (1,000 – 10,000 iterations using same tr. examples)
- Using net after training is fast
- Can overfitt

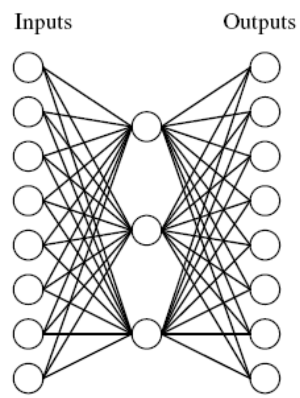
Representation power of FFNN

- Every boolean fct. can be repres. by a NN with one hidden layer (input x hidden x output ➔2 layers in total)

- NN with one hidden layer (input x hidden x output ➔ 2 layers in total) can approximate ANY continuous function (Cybenko'89, Hornik'89)

- NN with two hidden layers (input x hidden x hidden x output ➔ 3 layers in total) can approximate ANY function (Cybenko'88)

Ex.1 8-3-8 Binary encoder - decoder



- Hidden layer representation

→essential info from 8 ip. captured by 3 learned hidden units

→ability to invent features not explicitly introduced by humans

A target function:

Input		Output
10000000	→	10000000
01000000	→	01000000
00100000	→	00100000
00010000	→	00010000
00001000	→	00001000
00000100	→	00000100
00000010	→	00000010
00000001	→	00000001

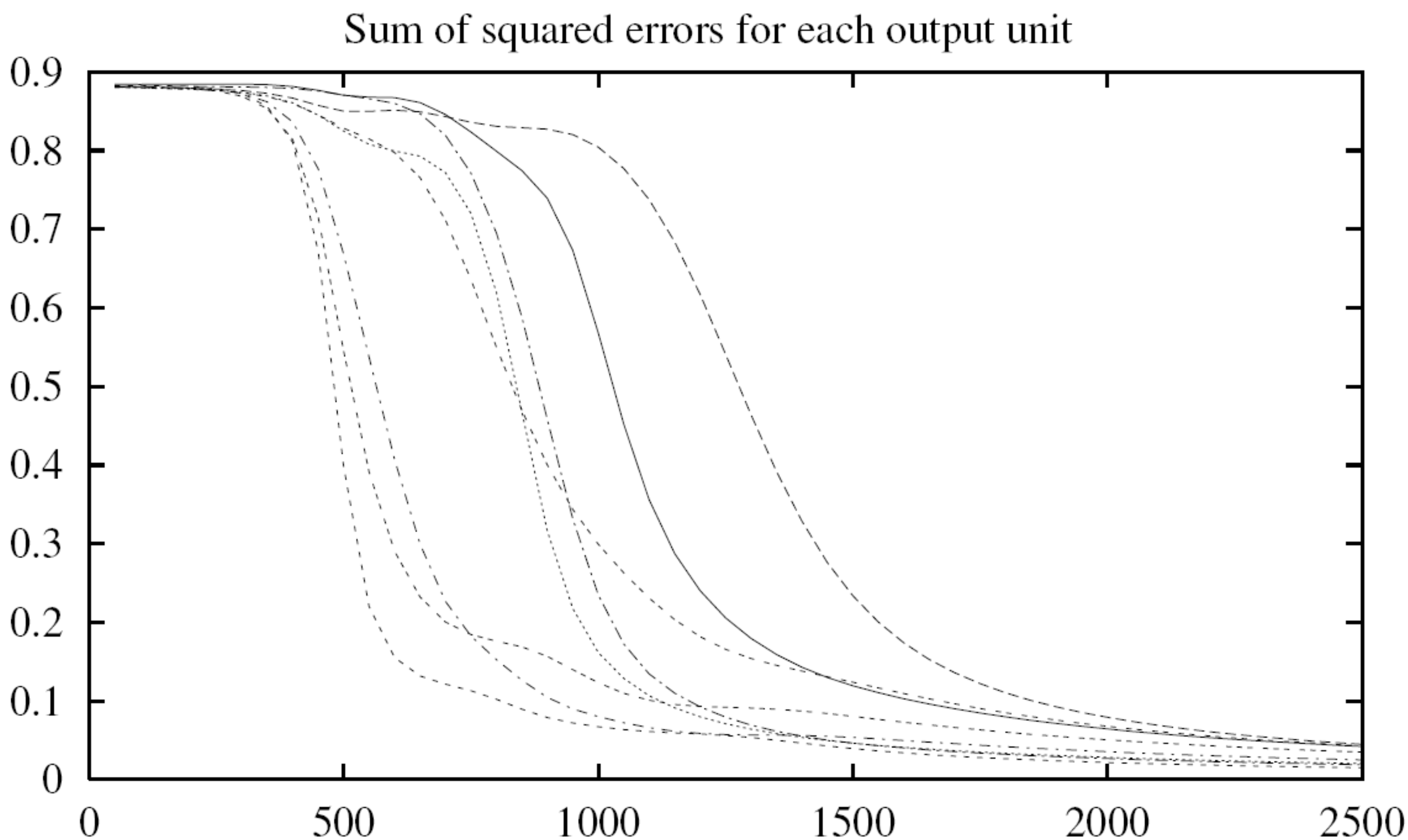
Can this be learned??

Learned hidden layer representation:

Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

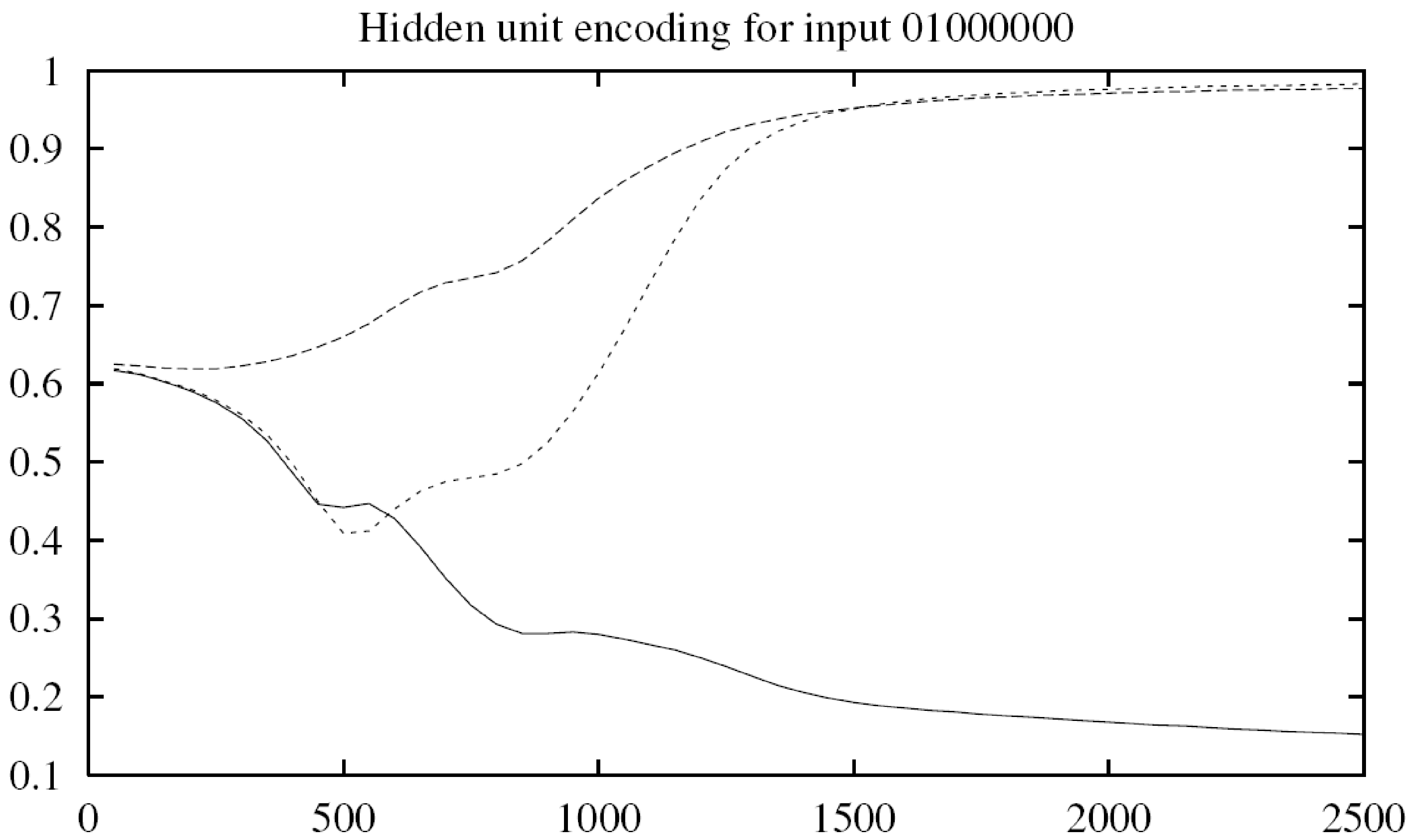
Training

- Sum of squared err for the 8 output units



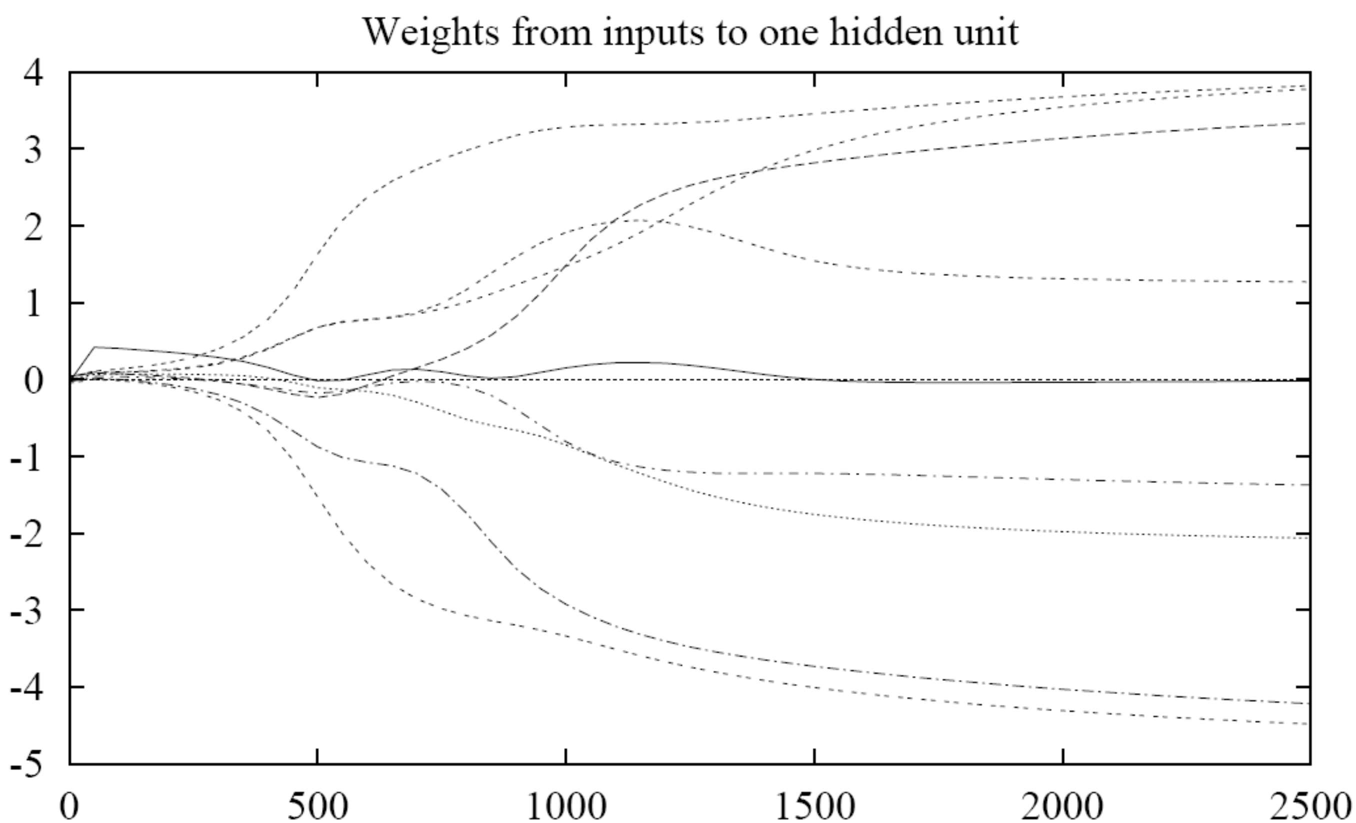
Training

- Hidden unit encoding for the 3 hidden units



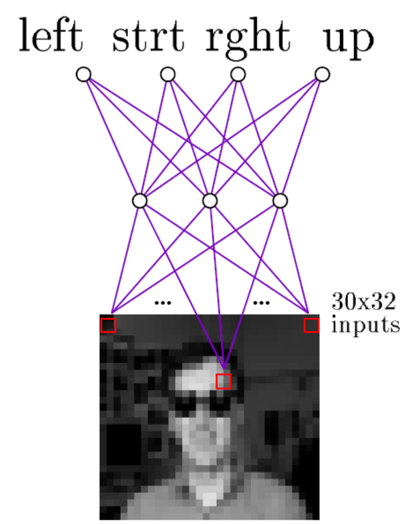
Training

- 9 weights from 8 ip. to 1 hidden unit



Ex.2 NN for face recognition

- Data
  - 624 greyscale images 120x128
  - Pixel intensity 0-255
- Task
  - predict forward, left, right, up
- Net
  - Ip: 30x32 pixel intensities
  - Op: 4 nodes
    (1-of-n op. coding) e.g.
    (.1,.1,.9,.1)
  - One hidden layer: 3 nodes
  - Tr. Time: 5 min to achieve 90% acc. (vs. 60 min for 30 hidden nodes which performs just slightly better (~92%))

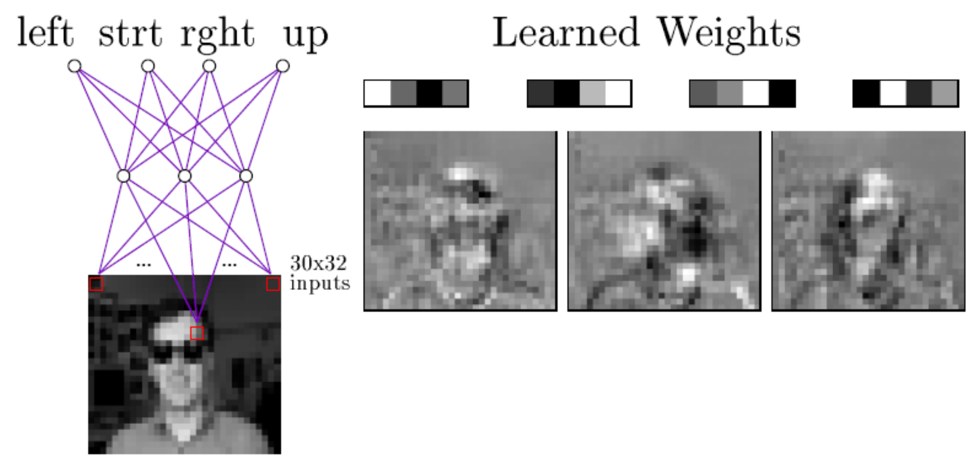


Typical input images

Ex.2 NN for face recognition

- Weights into the three hidden layer nodes after 100 epochs

- Weights from image pixels into each hidden unit, plotted in the pos. of the corresp. pixel



Typical input images

http://www.cs.cmu.edu/~tom/faces.html

Resources

- NN for Pattern Recognition, Bishop C.M., 1996

- Stuttgart NN Simulator (SNNS)

http://www.ra.cs.uni-tuebingen.de/SNNS/

- NN for face recognition

http://www.cs.cmu.edu/afs/cs.cmu.edu/user/mitchell/ftp/faces.html