

# Multi-Layer Artificial Neural Networks



## Chapter # 04 [Thomas Mitchel's Book] Learning Based Agents

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# Summary

Perceptron training rule guaranteed to succeed if

- Training examples are linearly separable
- Sufficiently small learning rate  $\eta$

Linear unit training rule uses gradient descent

- Guaranteed to converge to hypothesis with minimum squared error
- Given sufficiently small learning rate  $\eta$
- Even when training data contains noise
- Even when training data not separable by  $H$

# **Batch vs. Incremental Gradient Descent**

**Batch Mode** Gradient Descent:

Do until convergence

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 convergence

For each training example  $d$  in  $D$

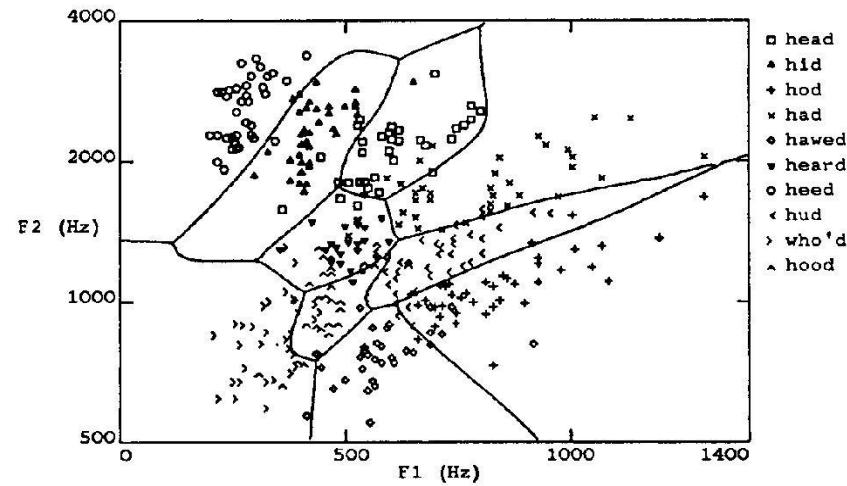
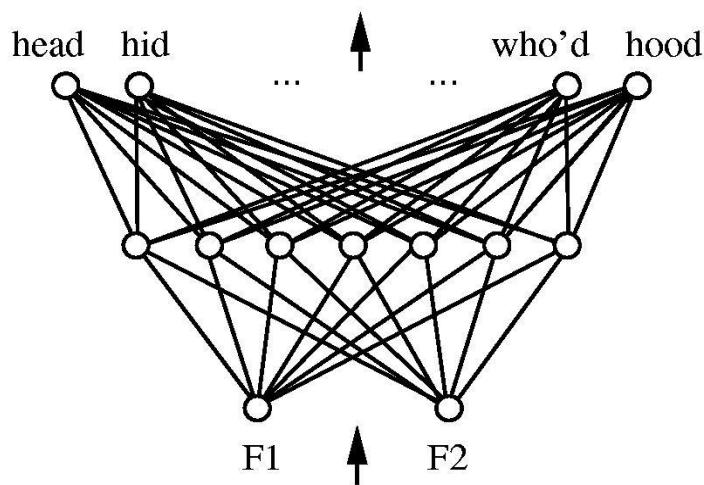
1. Compute the gradient  $\nabla E_d[\vec{w}]$
2.  $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$

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

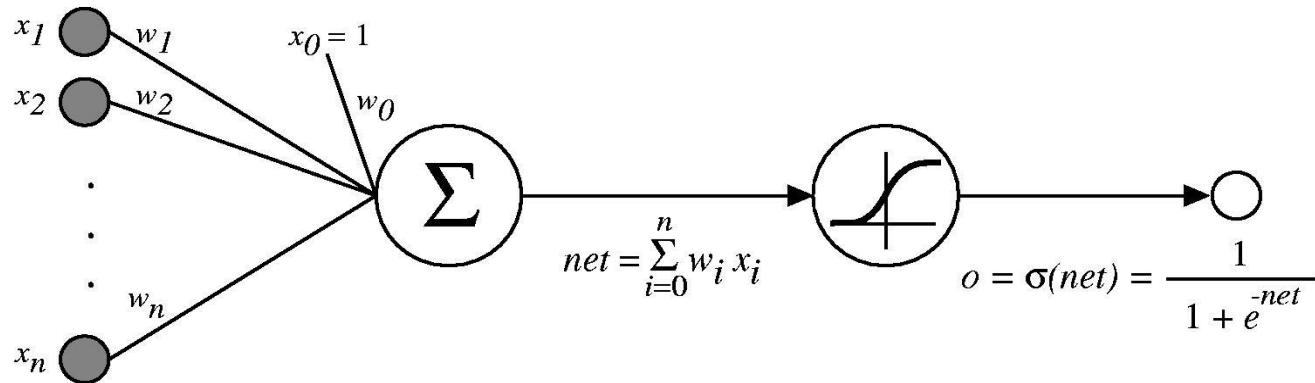
$$E_d[\vec{w}] \equiv \frac{1}{2} (t_d - o_d)^2$$

*Incremental Gradient Descent* can approximate *Batch Gradient Descent* arbitrarily closely if  $\eta$  made small enough

# Multilayer Networks of Sigmoid Units



# 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 descent rules to train

- One sigmoid unit
- *Multilayer networks* of sigmoid units → Backpropagation

## Error Gradient for a Sigmoid Unit

$$\begin{aligned}\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\ &= \sum_d (t_d - o_d) \left( -\frac{\partial o_d}{\partial w_i} \right) \\ &= -\sum_d (t_d - o_d) \frac{\partial o_d}{\partial net_d} \frac{\partial net_d}{\partial w_i}\end{aligned}$$

But we know:

$$\frac{\partial o_d}{\partial net_d} = \frac{\partial \sigma(net_d)}{\partial net_d} = o_d(1 - o_d)$$

$$\frac{\partial net_d}{\partial w_i} = \frac{\partial(\vec{w} \cdot \vec{x}_d)}{\partial w_i} = x_{i,d}$$

So:

$$\frac{\partial E}{\partial w_i} = - \sum_{d \in D} (t_d - o_d) o_d (1 - o_d) x_{i,d}$$

Let:  $\delta_k = -\frac{\partial E}{\partial net_k}$

$$\begin{aligned}
\frac{\partial E}{\partial net_j} &= \sum_{k \in Outs(j)} \frac{\partial E}{\partial net_k} \frac{\partial net_k}{\partial net_j} \\
&= \sum_{k \in Outs(j)} -\delta_k \frac{\partial net_k}{\partial net_j} \\
&= \sum_{k \in Outs(j)} -\delta_k \frac{\partial net_k}{\partial o_j} \frac{\partial o_j}{\partial net_j} \\
&= \sum_{k \in Outs(j)} -\delta_k w_{kj} \frac{\partial o_k}{\partial net_j} \\
&= \sum_{k \in Outs(j)} -\delta_k w_{kj} o_j (1 - o_j) \\
\delta_j &= -\frac{\partial E}{\partial net_j} = o_j (1 - o_j) \sum_{k \in Outs(j)} \delta_k w_{kj}
\end{aligned}$$

# Backpropagation Algorithm

Initialize all weights to small random numbers

Until convergence, Do

For each training example, Do

1. Input it to network and compute 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  $\Delta w_{i,j} = \eta \delta_j x_{i,j}$

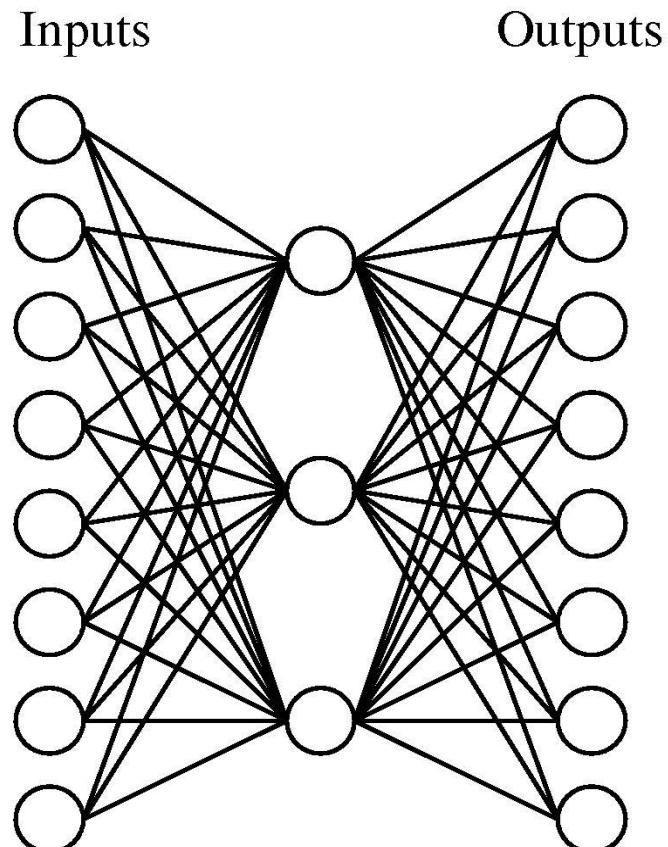
# More on Backpropagation

- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well  
(can run multiple times)
- Often include weight *momentum*  $\alpha$

$$\Delta w_{i,j}(n) = \eta \delta_j x_{i,j} + \alpha \Delta w_{i,j}(n - 1)$$

- Minimizes error over *training* examples
  - Will it generalize well to subsequent examples?
- Training can take thousands of iterations → slow!
- Using network after training is very fast

# Learning Hidden Layer Representations



A target function:

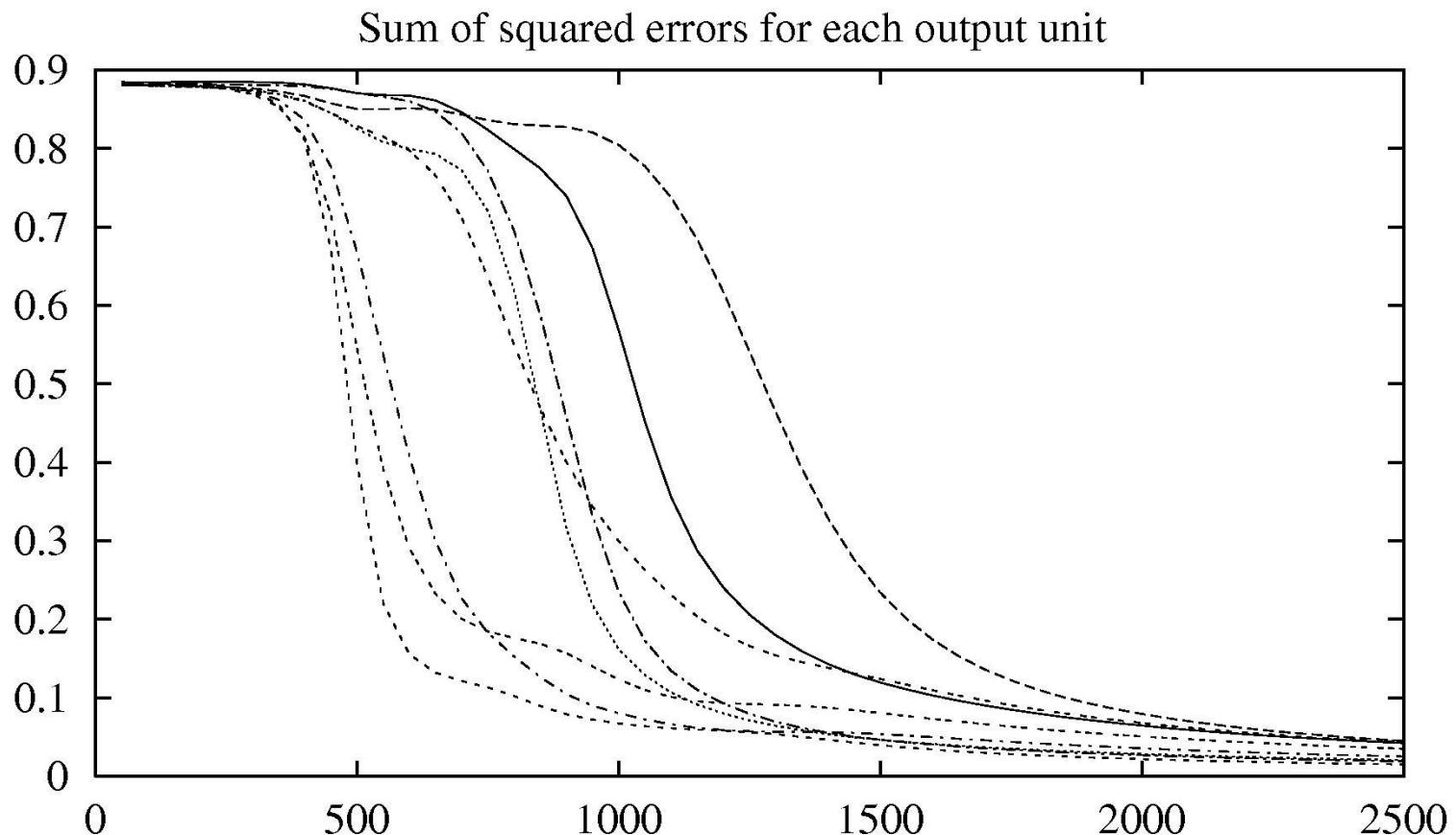
Input	Output
10000000	→ 10000000
01000000	→ 01000000
00100000	→ 00100000
00010000	→ 00010000
00001000	→ 00001000
00000100	→ 00000100
00000010	→ 00000010
00000001	→ 00000001

Can this be learned?

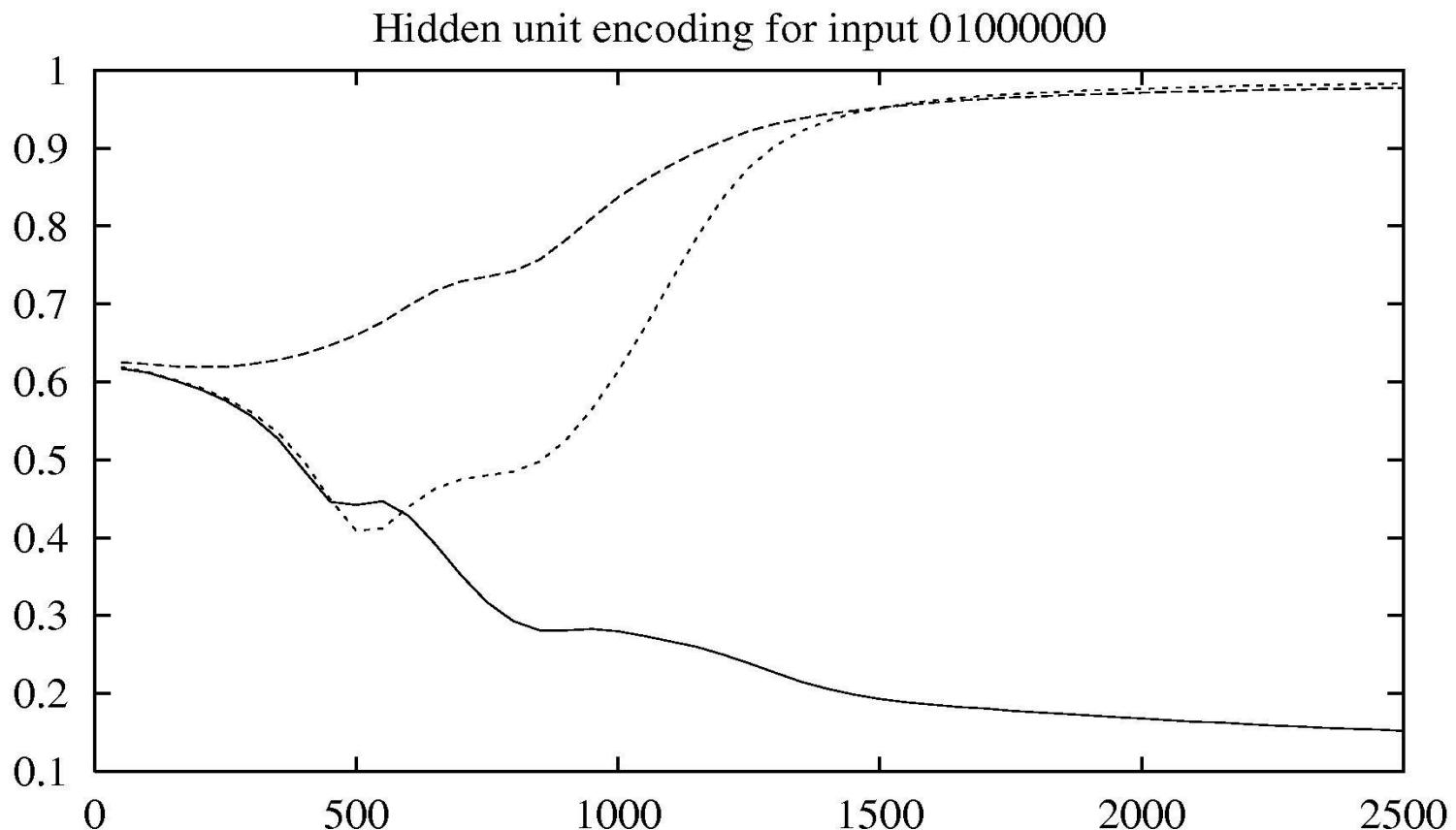
Learned hidden layer representation:

Input	Hidden Values			Output	
	.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

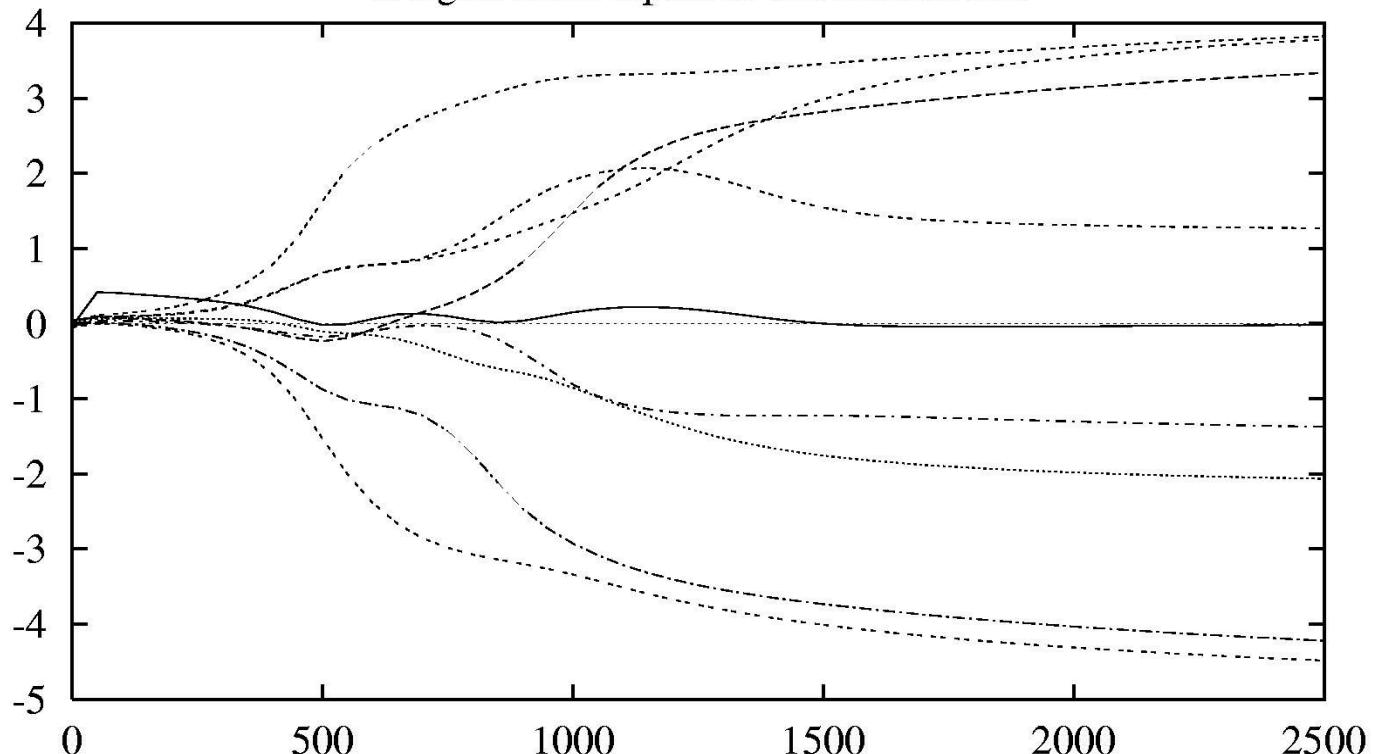


# Training



# Training

Weights from inputs to one hidden unit



# Convergence of Backpropagation

Gradient descent to some local minimum

- Perhaps not global minimum...
- Add momentum
- Stochastic gradient descent
- Train multiple nets with different initial weights

Nature of convergence

- Initialize weights near zero
- Therefore, initial networks near-linear
- Increasingly non-linear functions possible as training progresses

# Expressiveness of Neural Nets

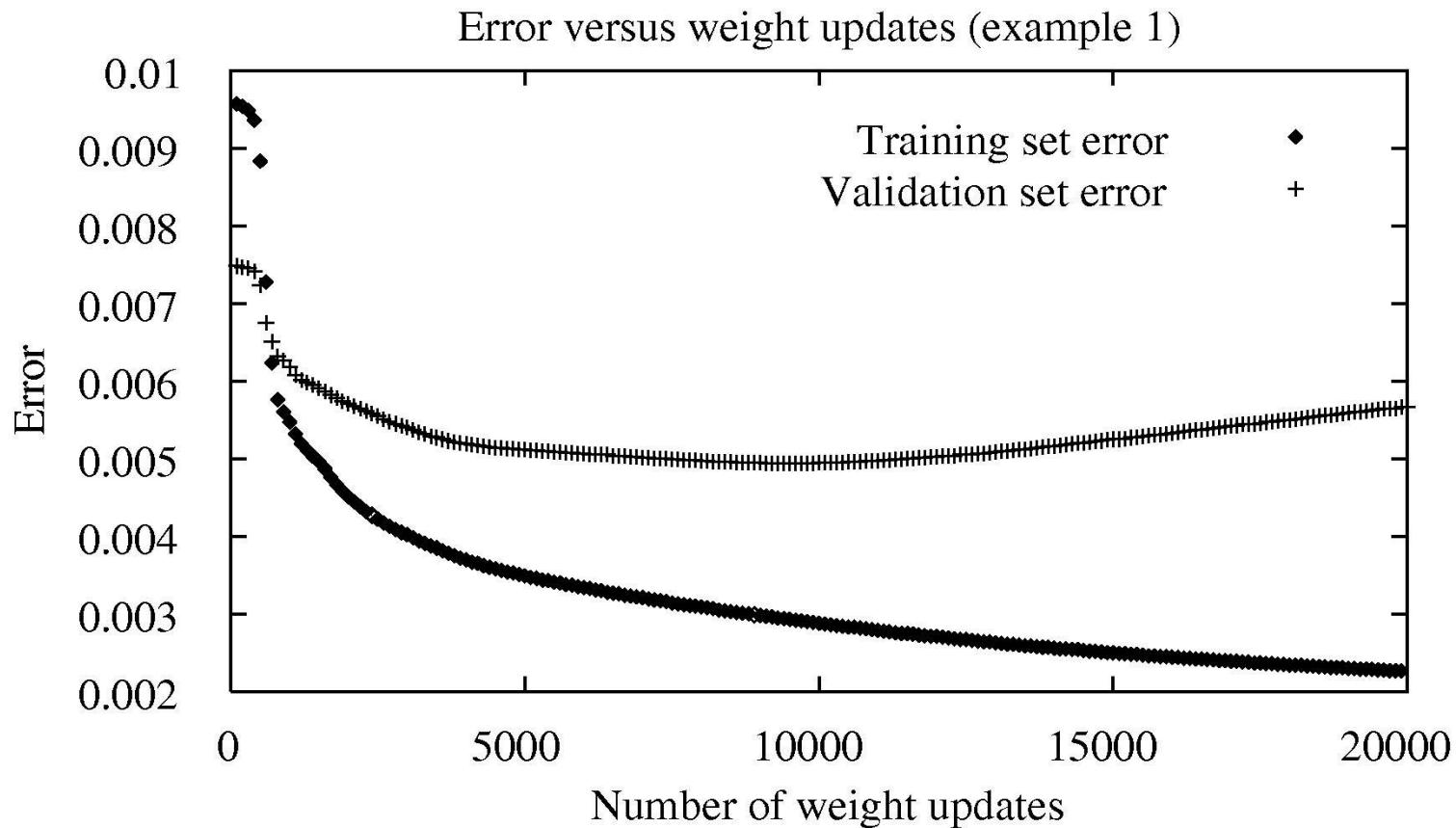
Boolean functions:

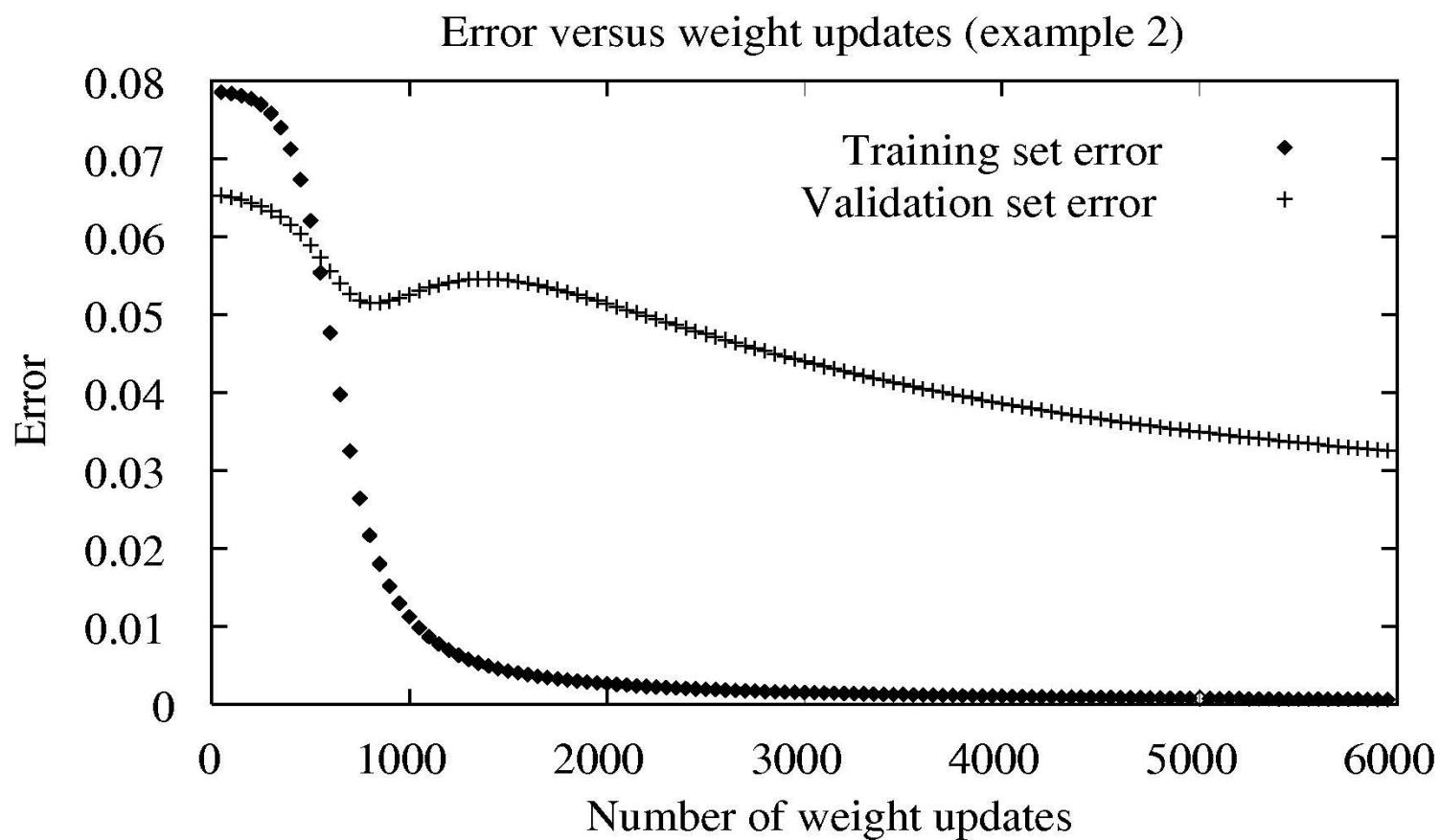
- Every Boolean function can be represented by network with single hidden layer
- But might require exponential (in number of inputs) hidden units

Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers

# Overfitting in Neural Nets





# Overfitting Avoidance

Penalize large weights:

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{kd} - o_{kd})^2 + \gamma \sum_{i,j} w_{ji}^2$$

Train on target slopes as well as values:

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} \left[ (t_{kd} - o_{kd})^2 + \mu \sum_{j \in inputs} \left( \frac{\partial t_{kd}}{\partial x_d^j} - \frac{\partial o_{kd}}{\partial x_d^j} \right)^2 \right]$$

Weight sharing

Early stopping

# Neural Networks: Summary

- Perceptrons
- Gradient descent
- Multilayer networks
- Backpropagation