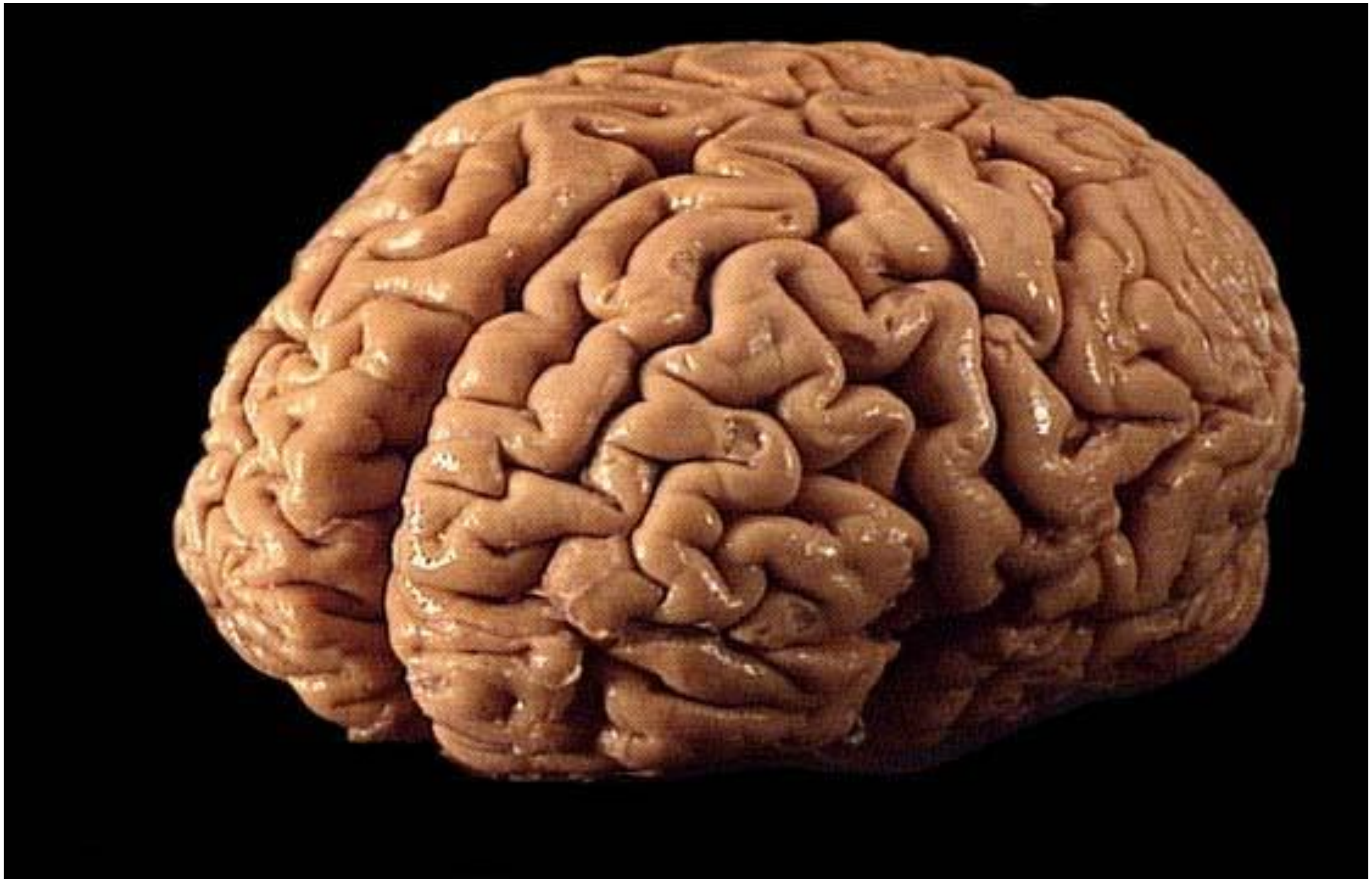
Machine Learning

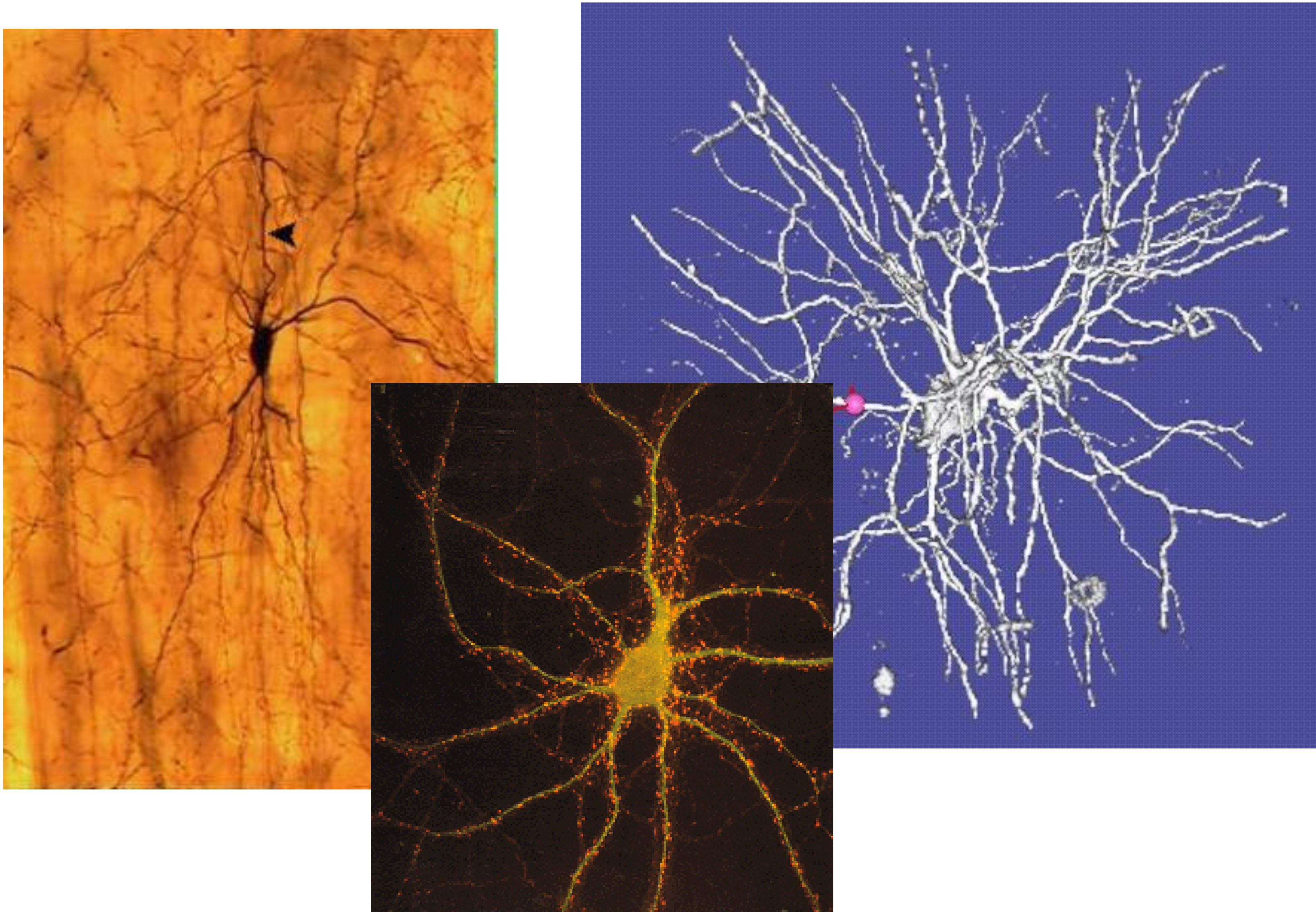
Neural Networks

(slides from Domingos, Pardo, others)

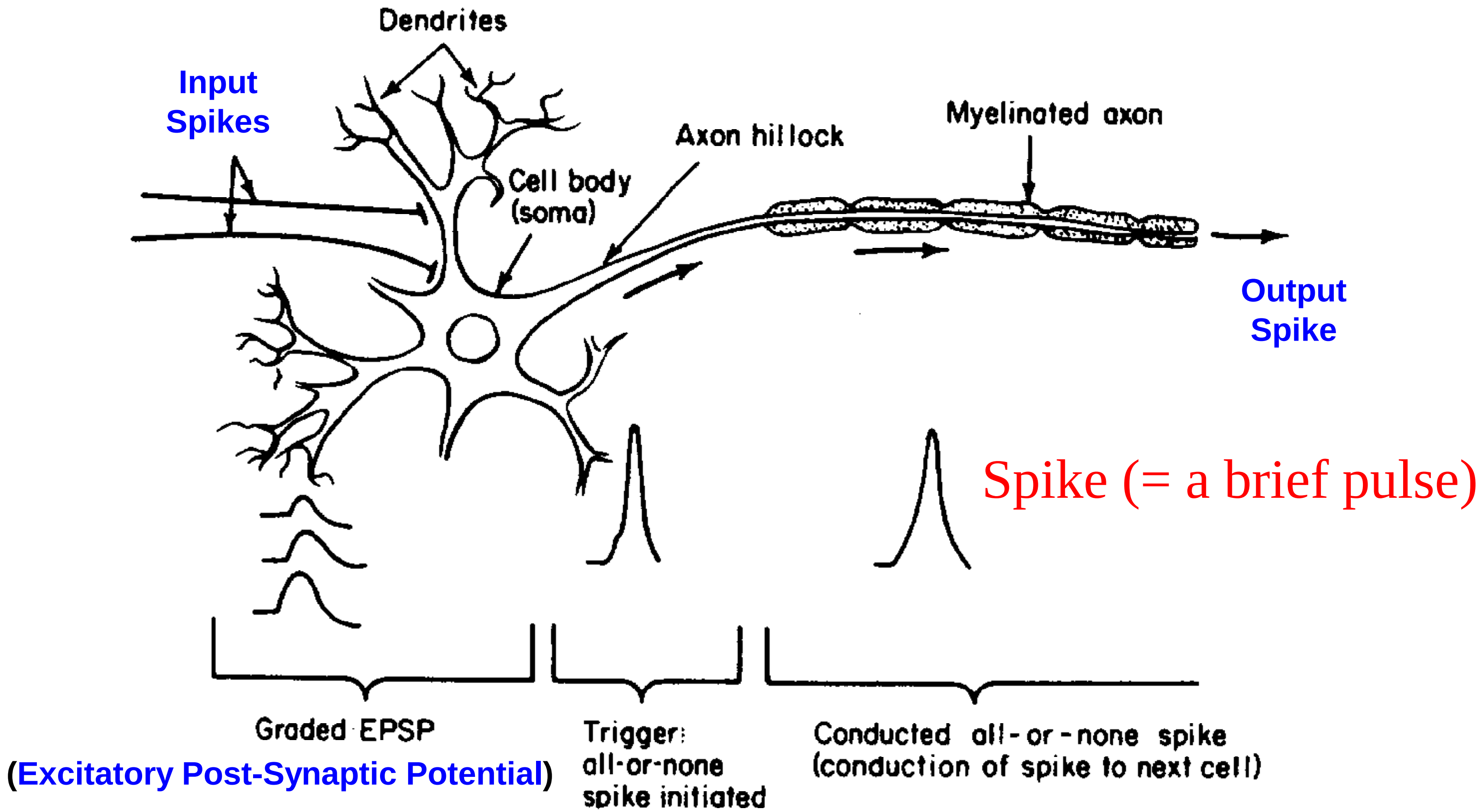
Human Brain



Neurons



Input-Output Transformation

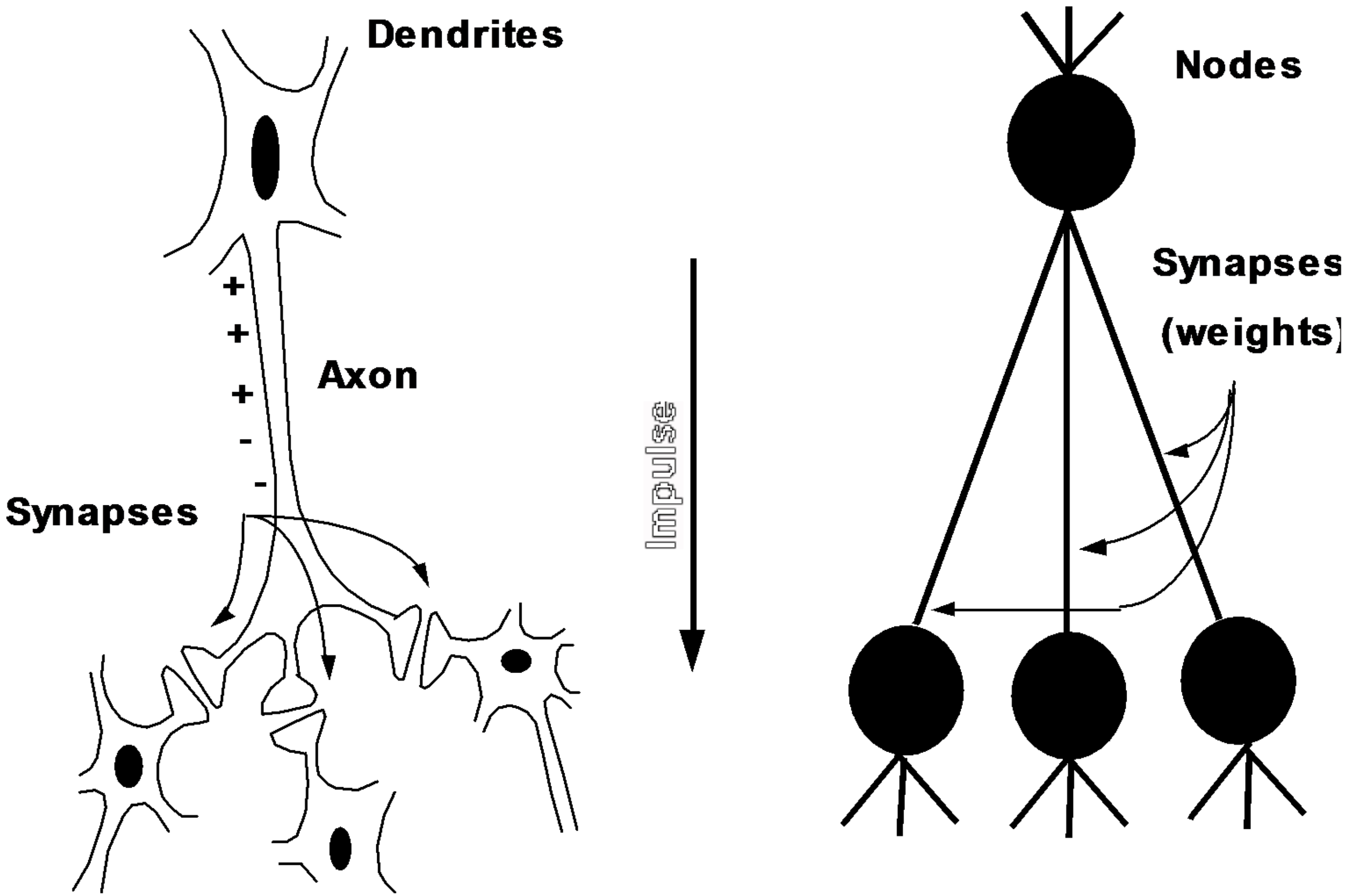


Human Learning

- Number of neurons: ~ 10^{11}
- Connections per neuron: ~ 10^3 to 10^5
- Neuron switching time: ~ 0.001 second
- Scene recognition time: ~ 0.1 second

100 inference steps doesn't seem much

Machine Learning Abstraction



Artificial Neural Networks

- Typically, machine learning ANNs are very artificial, ignoring:
  - Time
  - Space
  - Biological learning processes
- More realistic neural models exist
  - Hodgkin & Huxley (1952) won a Nobel prize for theirs (in 1963)
- Nonetheless, very artificial ANNs have been useful in many ML applications

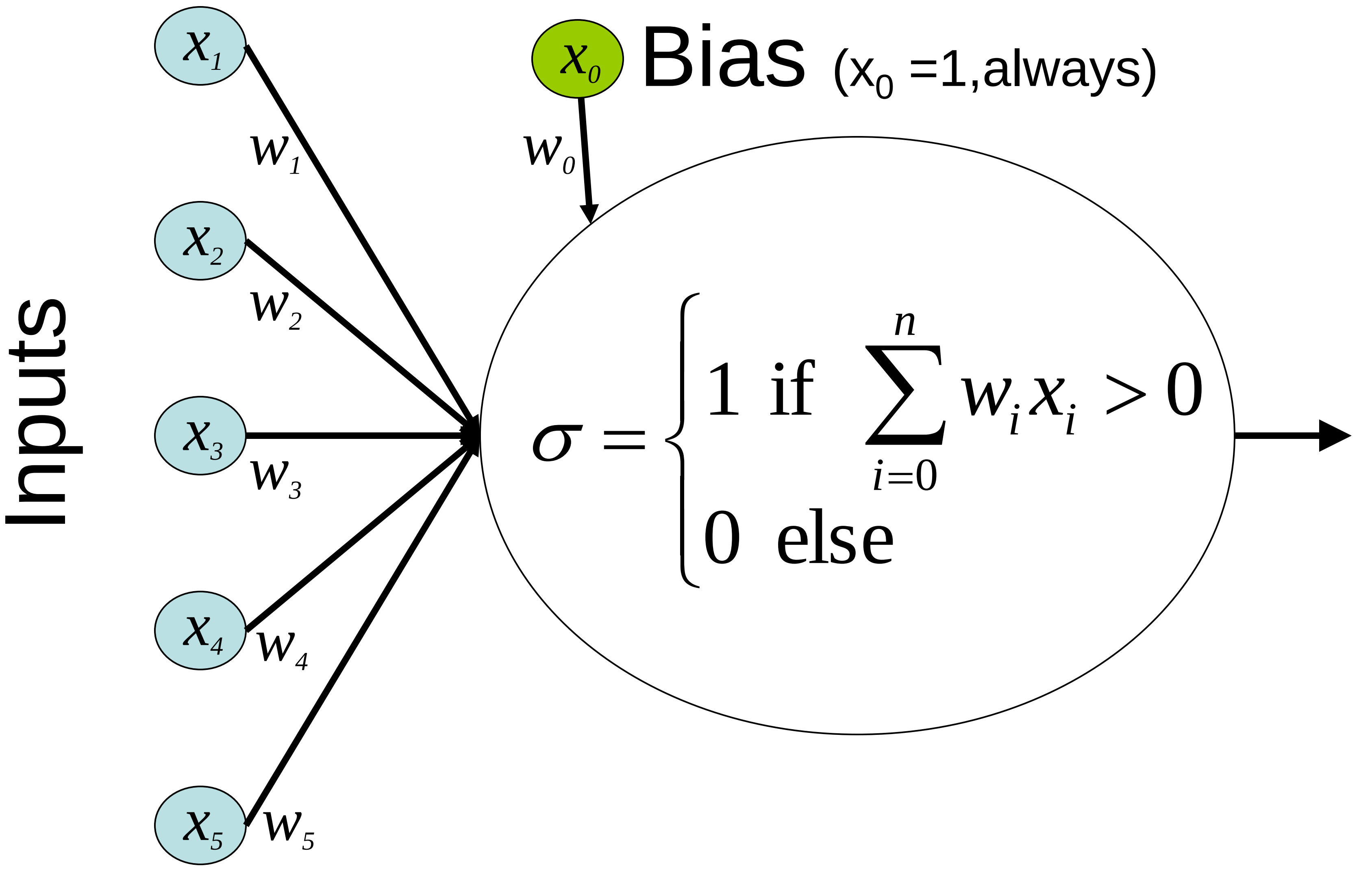
Perceptrons

- The “first wave” in neural networks
- Big in the 1960’s
  - McCulloch & Pitts (1943), Woodrow & Hoff (1960), Rosenblatt (1962)

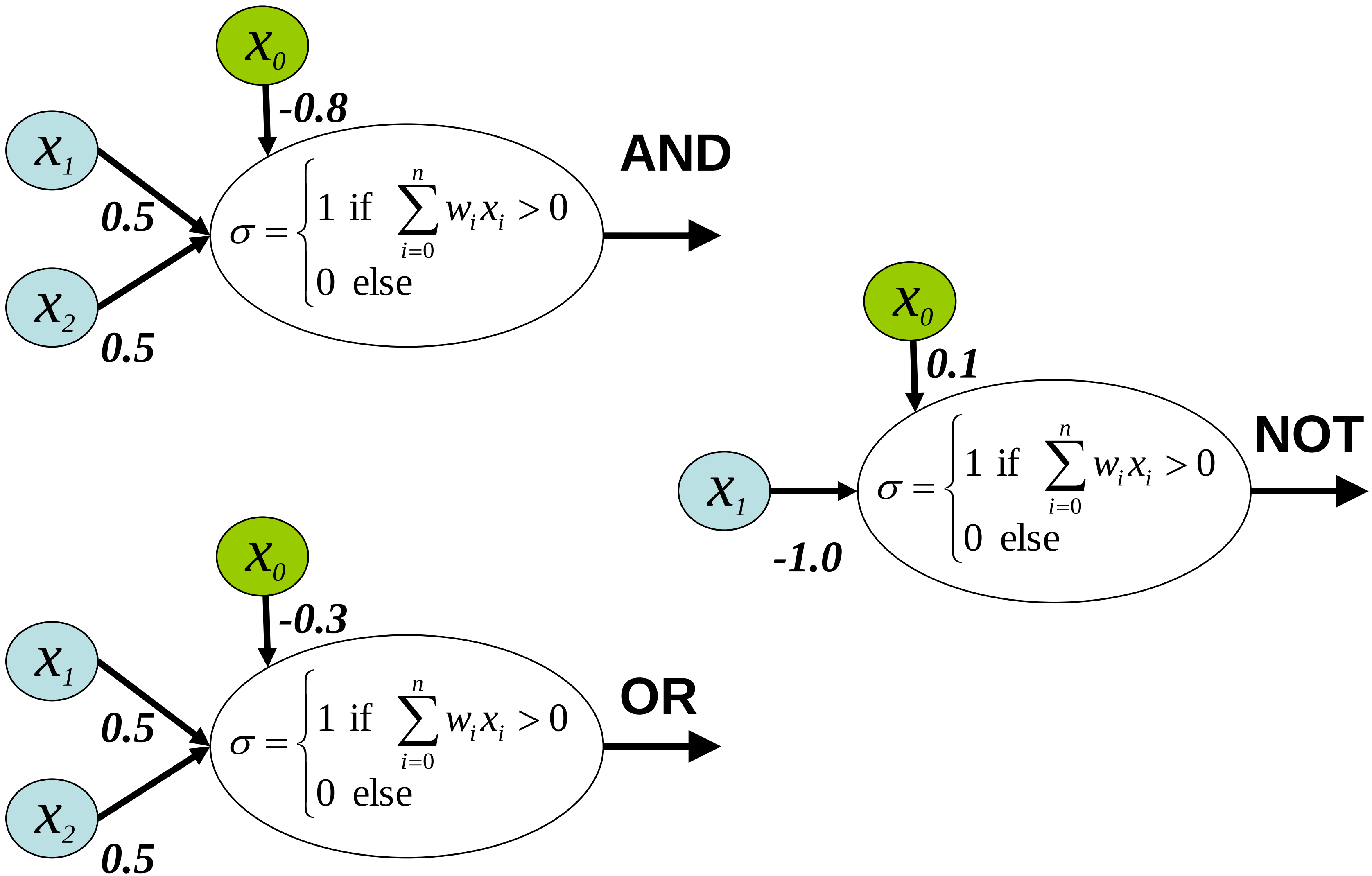
Perceptrons

- Problem def:
  - Let f be a target function from $X = \langle x_1, x_2, \ldots \rangle$ where $x_i \in \{0, 1\}$ to $y \in \{0, 1\}$
  - Given training data $\{(X_1, y_1), (X_2, y_2) \ldots\}$
    - Learn $h(X)$, an approximation of $f(X)$

A single perceptron

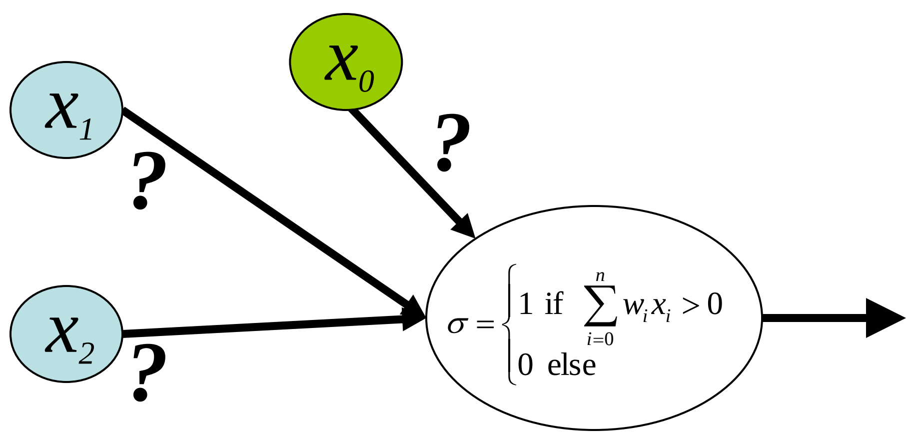


Logical Operators



Learning Weights

- Perceptron Training Rule
- Gradient Descent
- (other approaches: Genetic Algorithms)



Perceptron Training Rule

- Weights modified for each training example
- Update Rule:

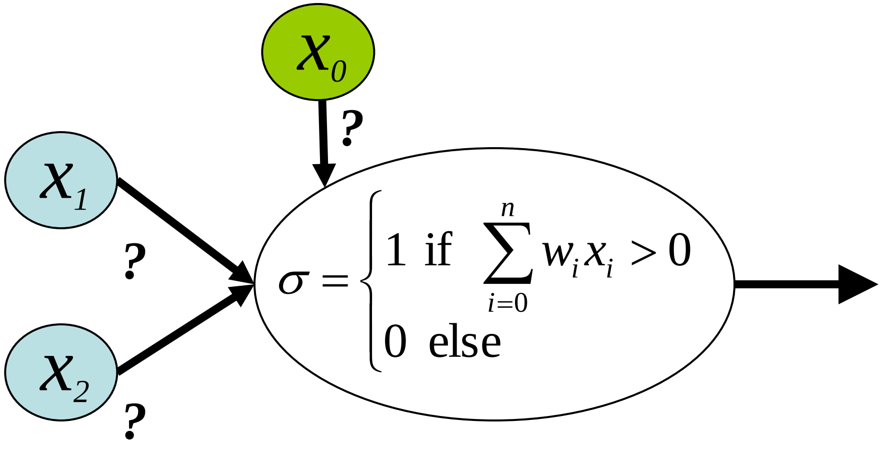
$$w_i \leftarrow w_i + \Delta w_i$$

where

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

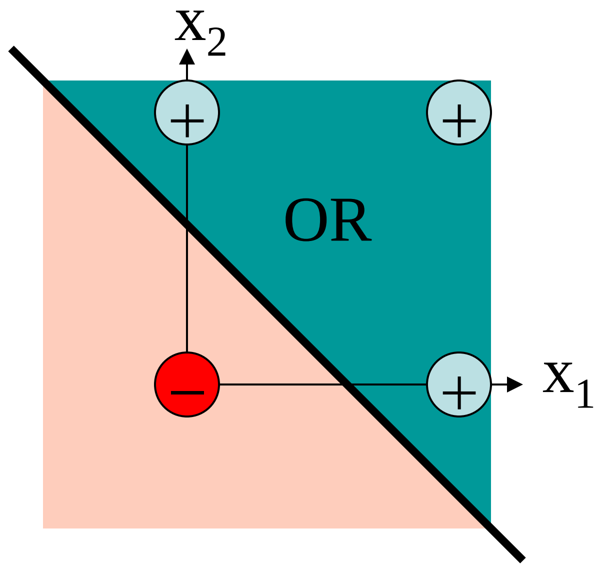
learning rate | target value | perceptron output | input value

What weights make XOR?

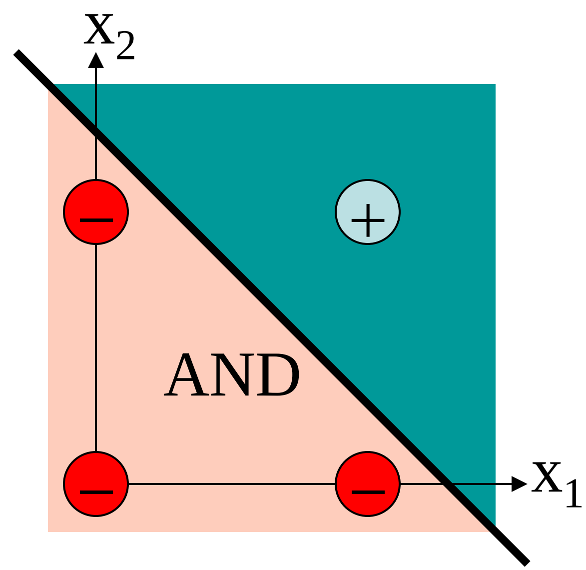


- No combination of weights works
- Perceptrons can only represent linearly separable functions

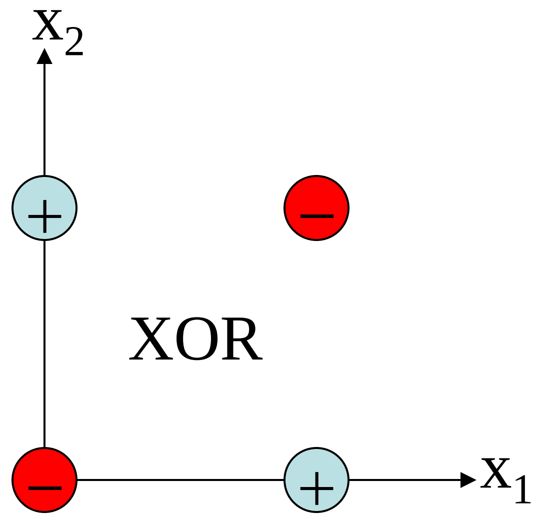
Linear Separability



Linear Separability



Linear Separability

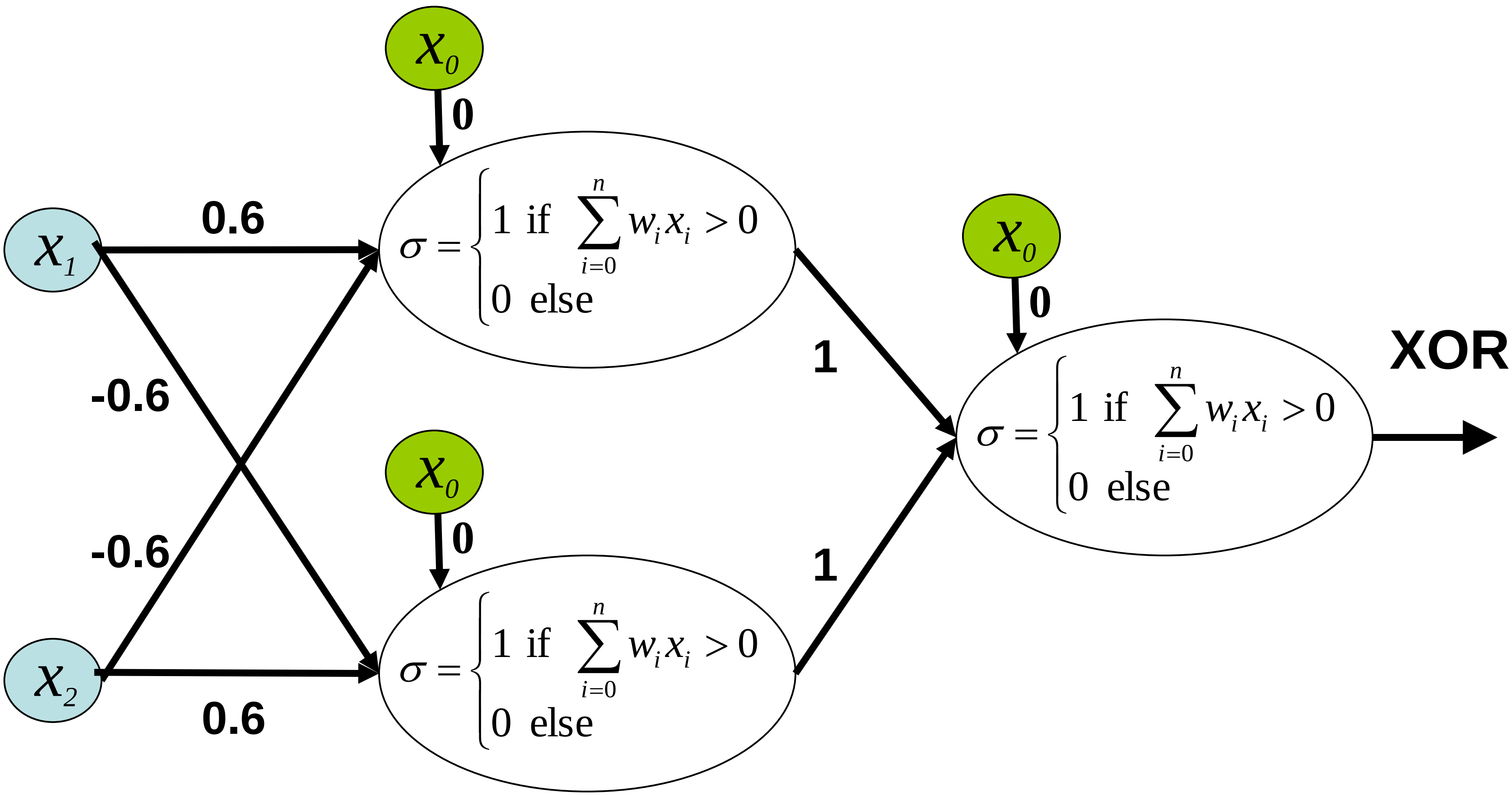


Perceptron Training Rule

- Converges to the correct classification IF
  - Cases are linearly separable
  - Learning rate is slow enough
  - Proved by Minsky and Papert in 1969

Killed widespread interest in perceptrons till the 80's

XOR

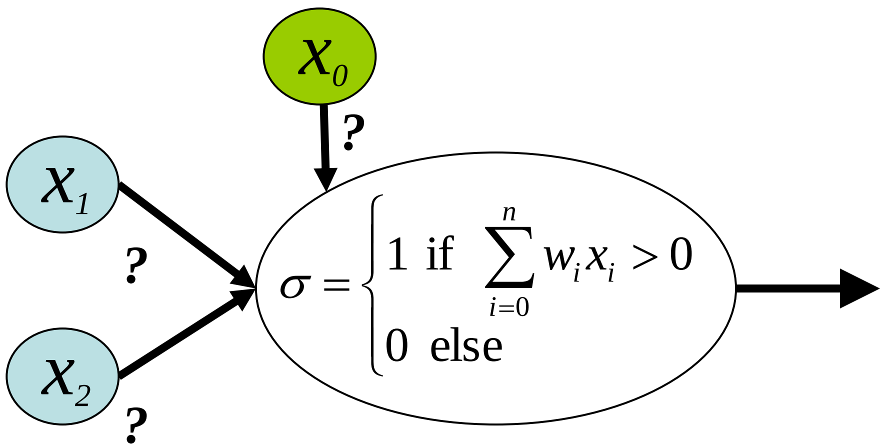


x_0
0
x_0
0
x_0
0
x_1
x_2
0.6
-0.6
-0.6
0.6
$\sigma = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ 0 \text{ else} \end{cases}$
$\sigma = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ 0 \text{ else} \end{cases}$
1
1
$\sigma = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ 0 \text{ else} \end{cases}$
XOR

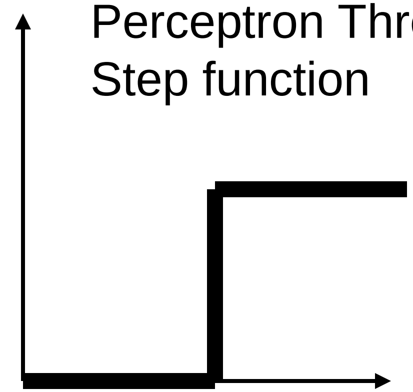
What's wrong with perceptrons?

- You can always plug multiple perceptrons together to calculate any function.
- BUT…who decides what the weights are?
  - Assignment of error to parental inputs becomes a problem….
  - This is because of the threshold….
    - Who contributed the error?

Perceptrons use a step function

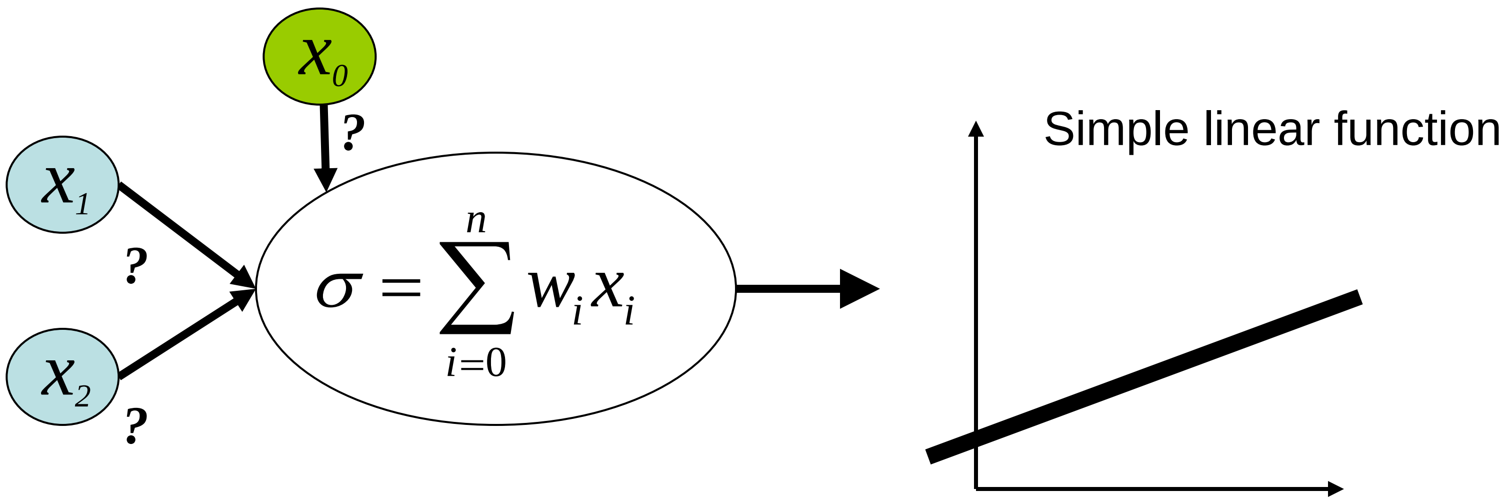


Perceptron Threshold
Step function



- Small changes in inputs -> either no change or large change in output.

Solution: Differentiable Function



- Varying any input a little creates a perceptible change in the output
- We can now characterize how *error* changes w_i even in multi-layer case

Measuring error for linear units

- Output Function

$$\sigma(\vec{x}) = \vec{w} \cdot \vec{x}$$

- Error Measure:

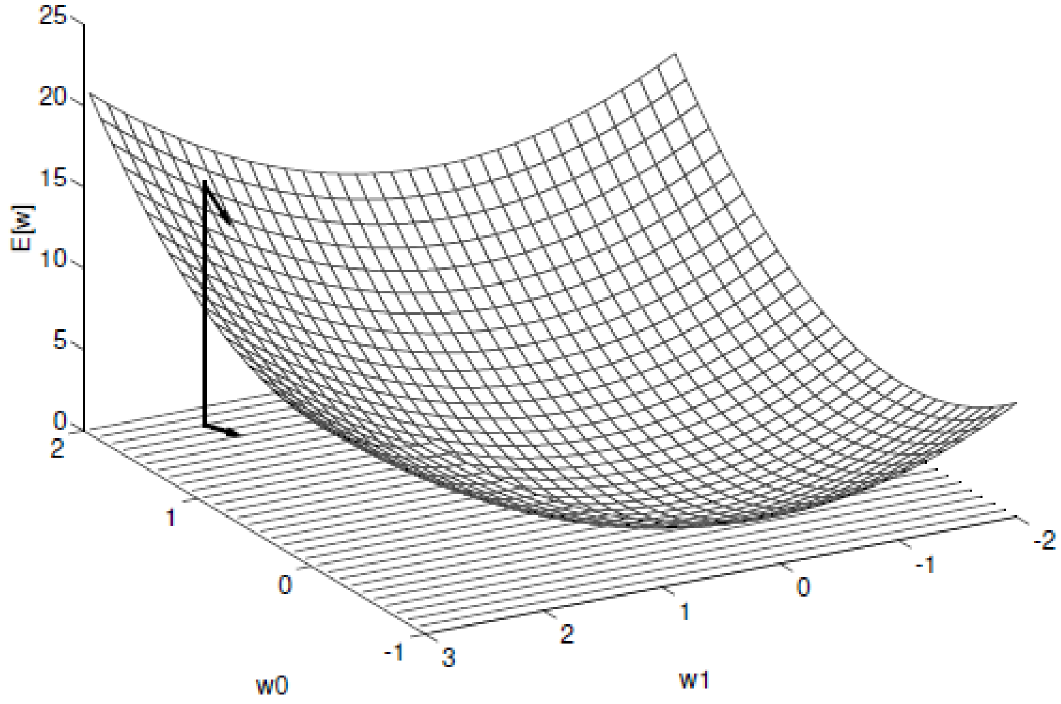
$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

data

target value

linear unit output

Gradient Descent



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:

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

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

Gradient Descent Rule

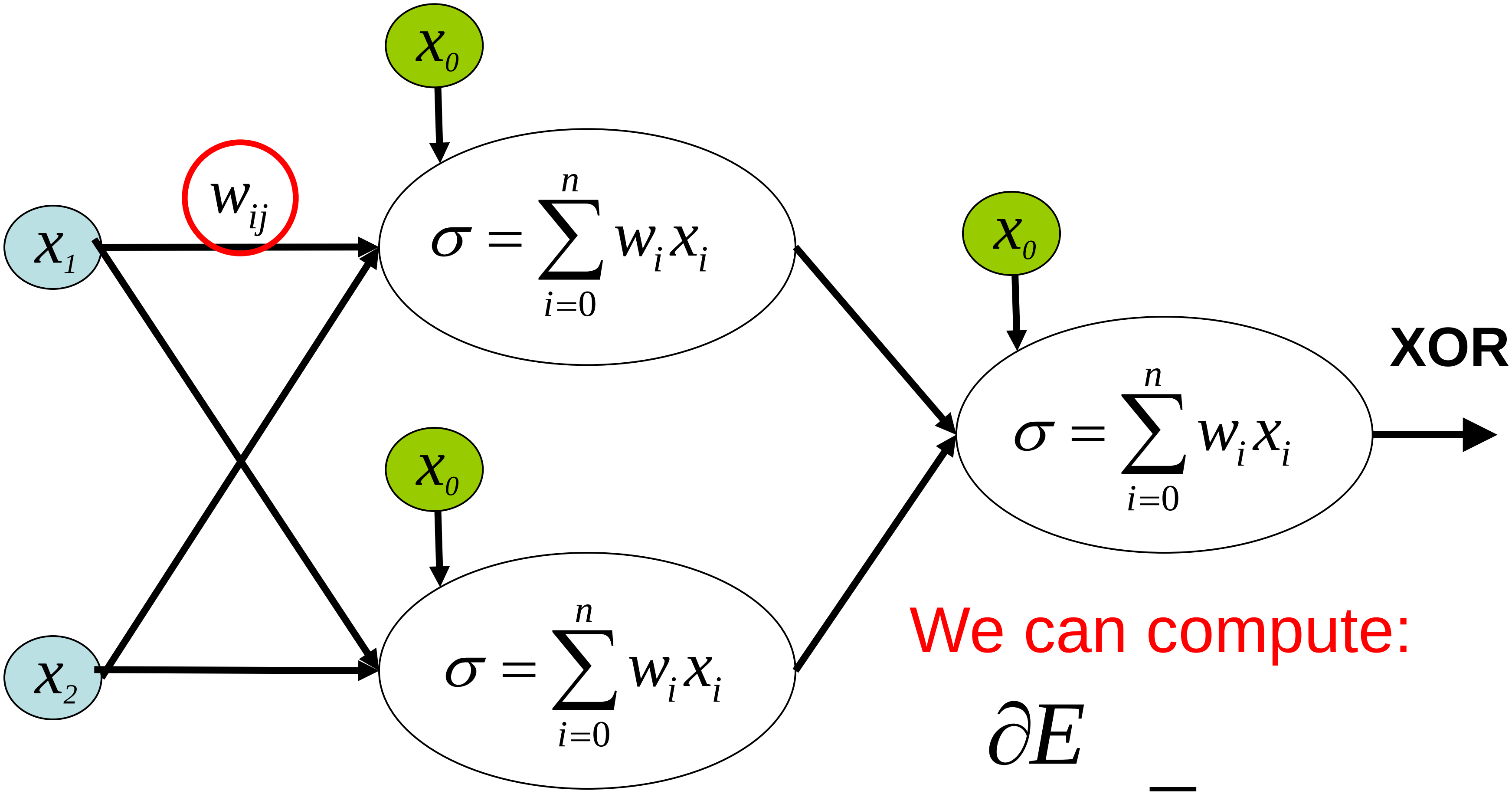
$$\frac{\partial E}{\partial w_i} \equiv \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$$

$$= \sum_{d \in D} (t_d - o_d)(-x_{i,d})$$

Update Rule:

$$w_i \leftarrow w_i + \eta \sum_{d \in D} (t_d - o_d) x_{i,d}$$

Gradient Descent for Multiple Layers



We can compute:

$$\frac{\partial E}{\partial w_{ij}} = \ldots$$

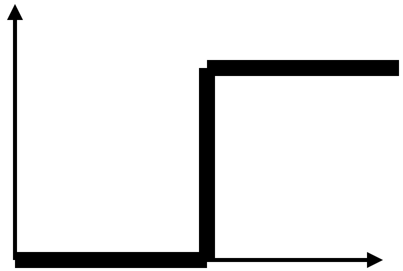
Gradient Descent vs. Perceptrons

- Perceptron Rule & Threshold Units
  - Learner converges on an answer ONLY IF data is linearly separable
  - Can't assign proper error to parent nodes
- Gradient Descent
  - (locally) Minimizes error even if examples are not linearly separable
  - Works for multi-layer networks
    - But…linear units only make linear decision surfaces (can't learn XOR even with many layers)
  - And the step function isn't differentiable…

A compromise function

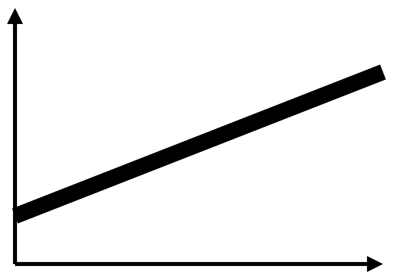
- Perceptron

$$output = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ 0 \text{ else} \end{cases}$$



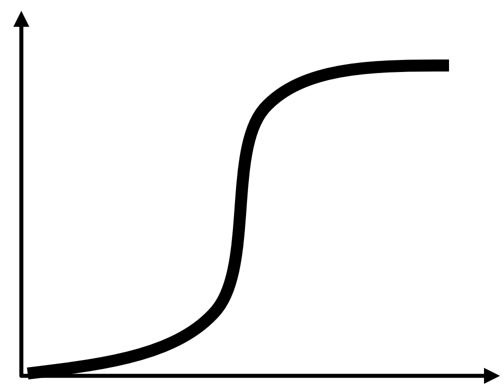
- Linear

$$output = net = \sum_{i=0}^{n} w_i x_i$$



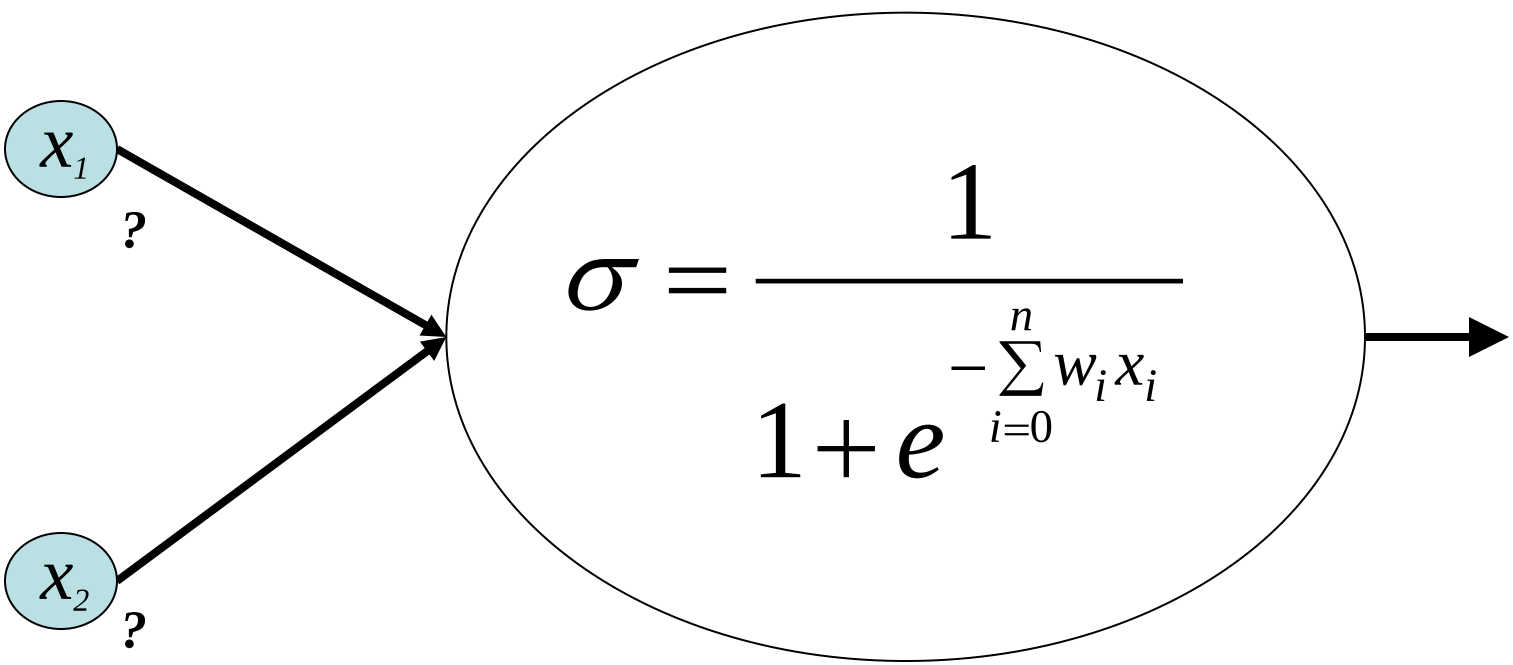
- Sigmoid (Logistic)

$$output = \sigma(net) = \frac{1}{1+e^{-net}}$$

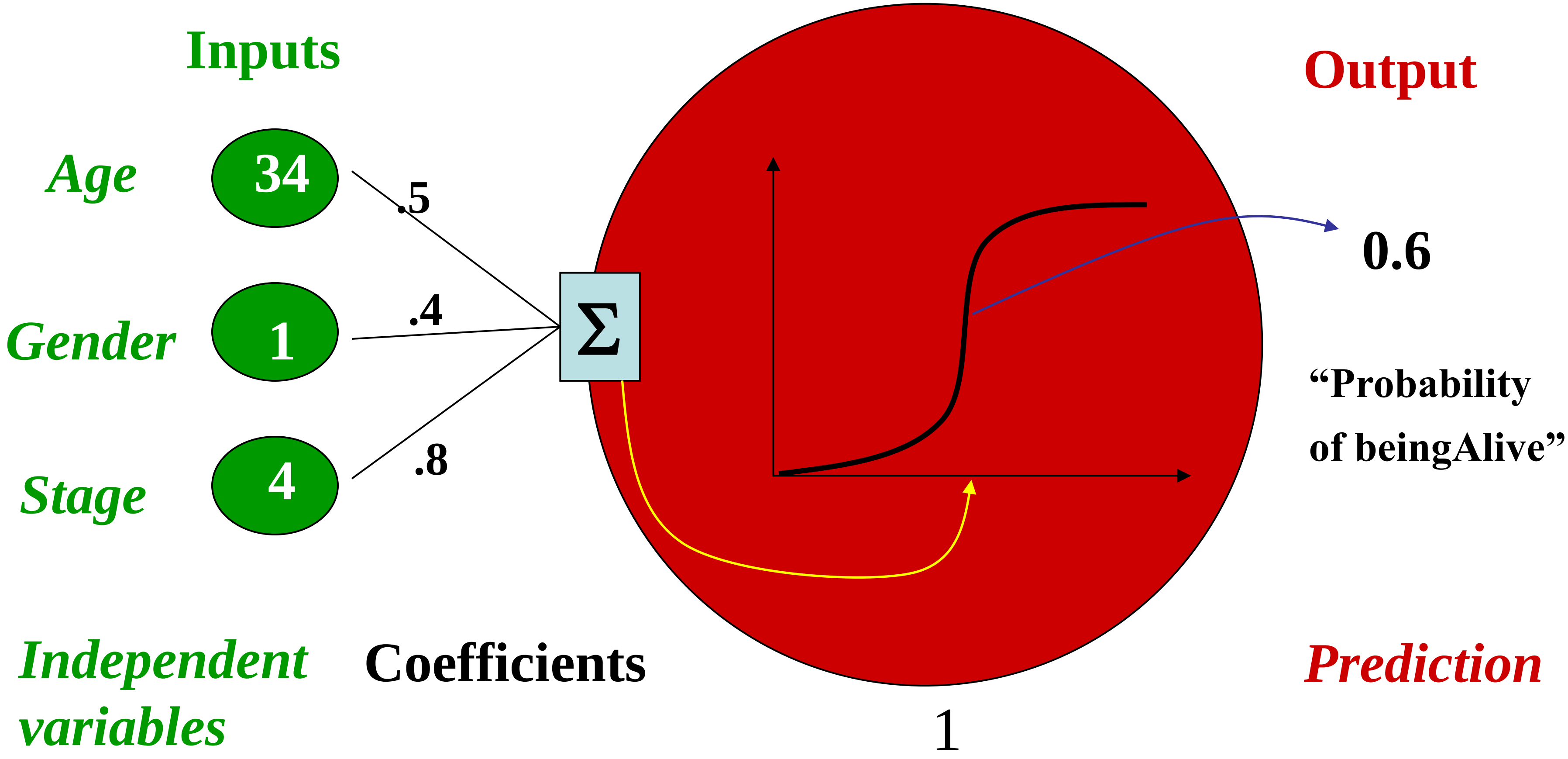


The sigmoid (logistic) unit

- Has differentiable function
  - Allows gradient descent
- Can be used to learn non-linear functions

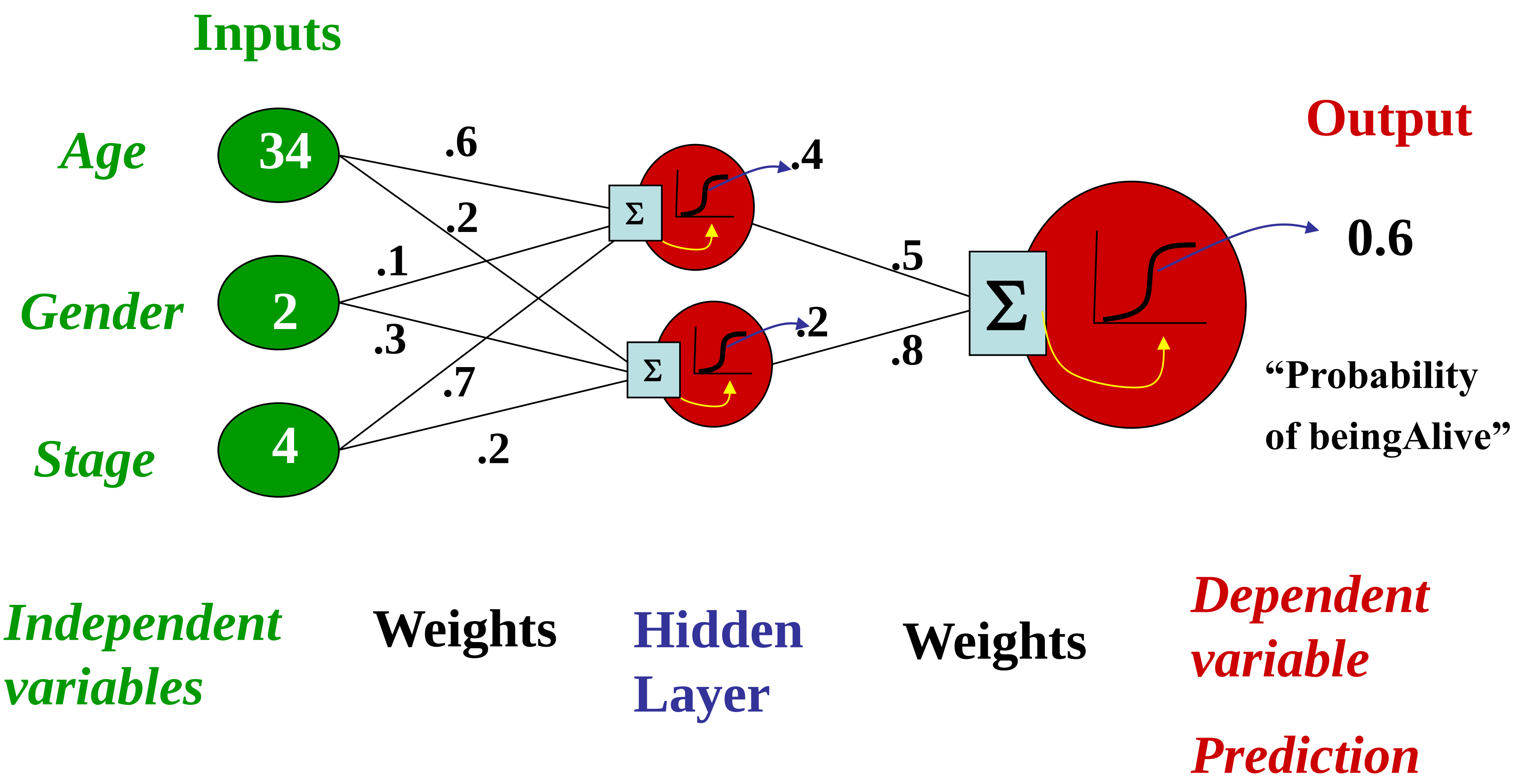


Logistic function

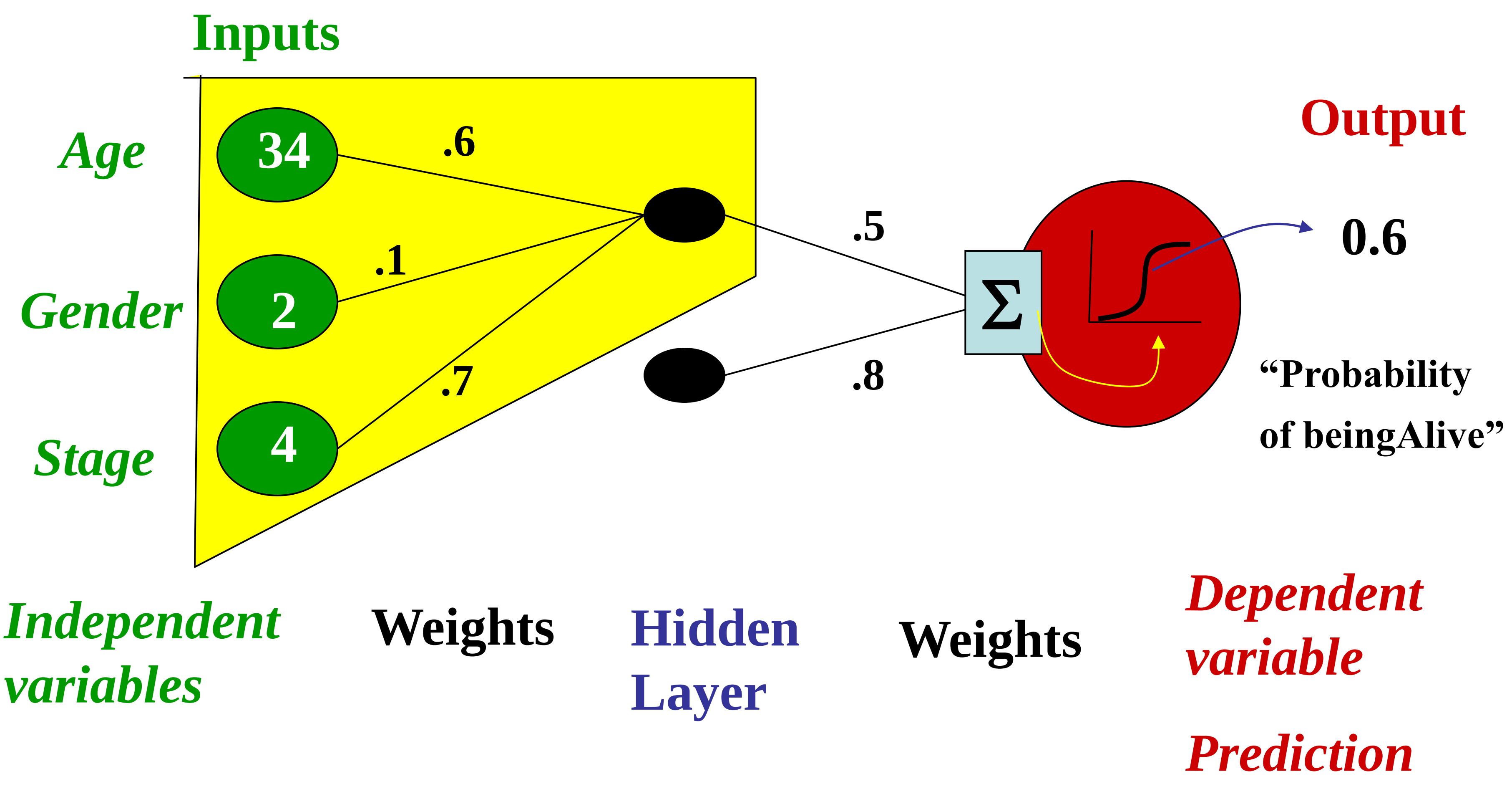


$$\sigma = \frac{1}{1 + e^{-\sum_{i=0}^{n} w_i x_i}}$$

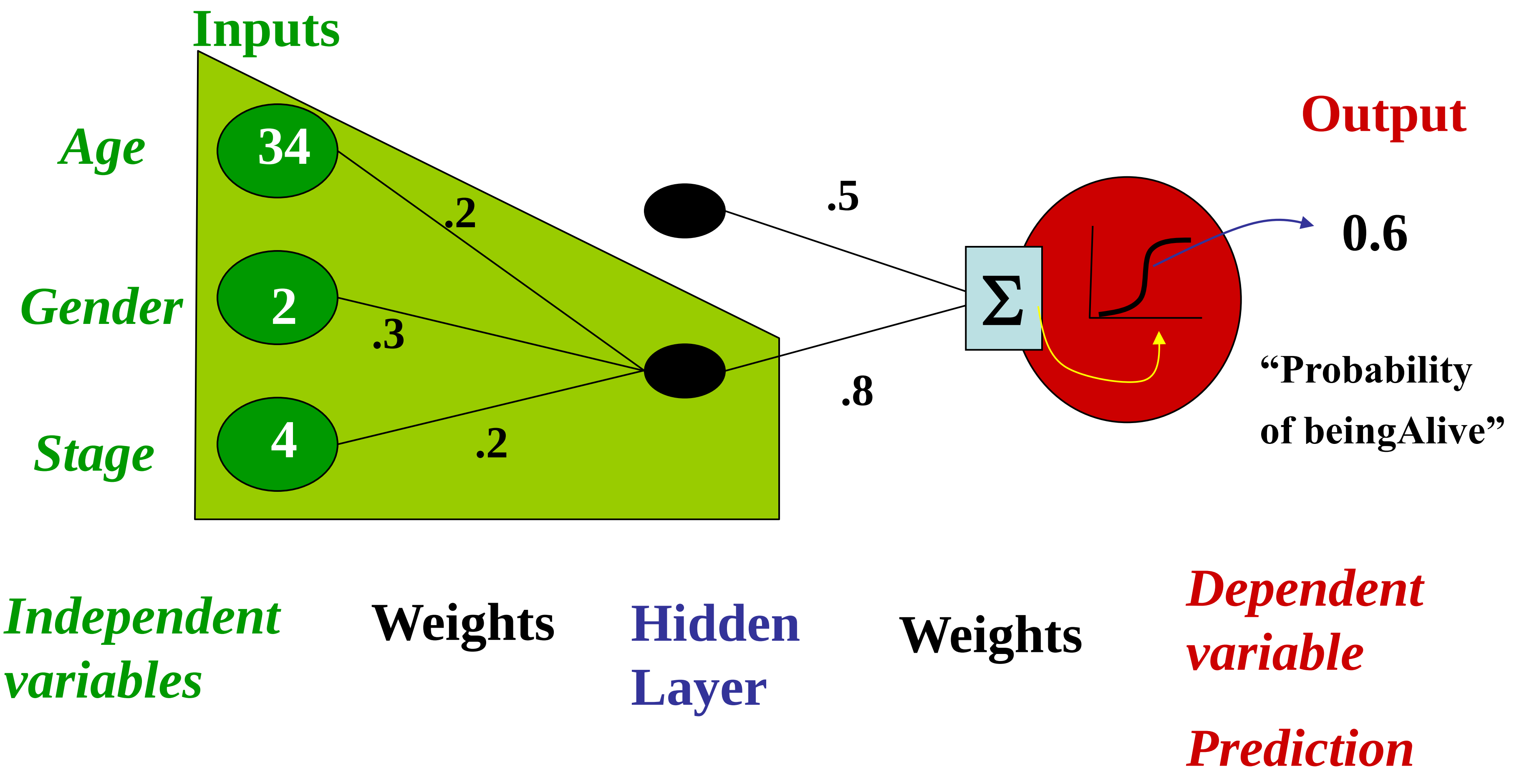
Neural Network Model



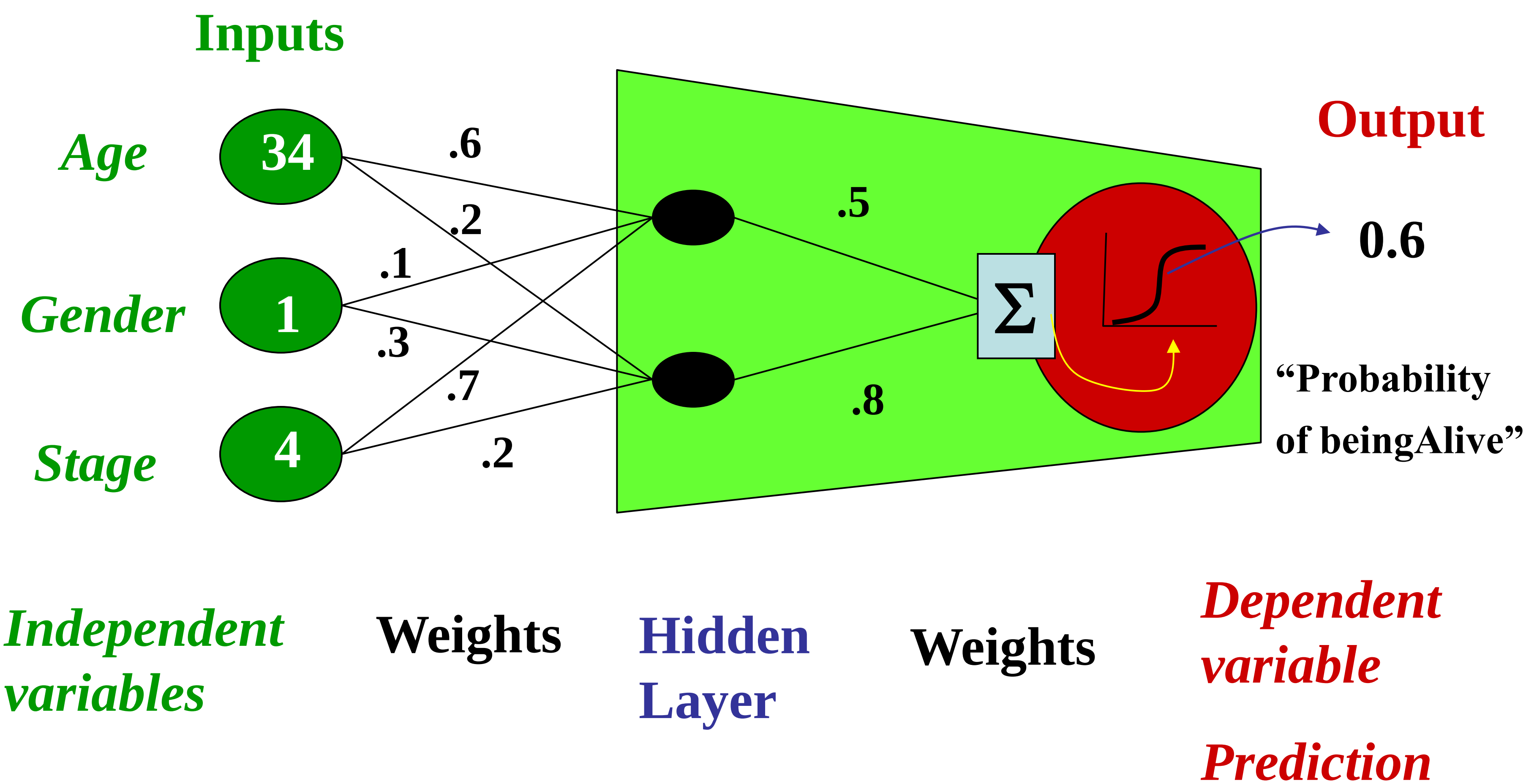
Getting an answer from a NN



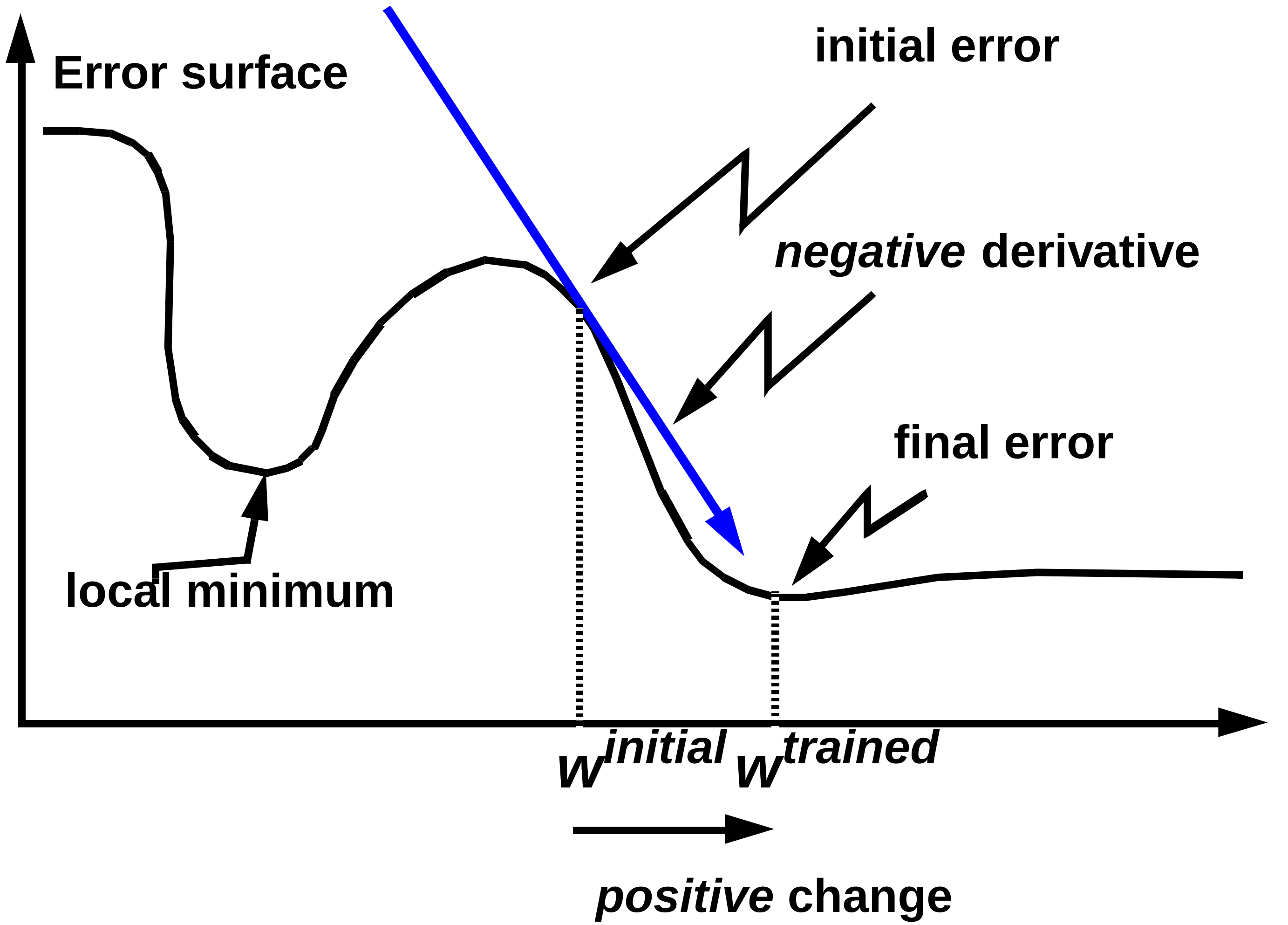
Getting an answer from a NN



Getting an answer from a NN



Minimizing the Error



Differentiability is key!

- Sigmoid is easy to differentiate

$$\frac{\partial \sigma(y)}{\partial y} = \sigma(y) \cdot (1 - \sigma(y))$$

- For gradient descent on multiple layers, a little dynamic programming can help:
  - Compute errors at each output node
  - Use these to compute errors at each hidden node
  - Use these to compute errors at each input node

The Backpropagation Algorithm

For each input training example, $\left\langle \vec{x}, \vec{t} \right\rangle$

1. Input instance $\vec{x}$ to the network and compute the output o_u for every unit u in the network

2. For each output unit k, calculate its error term δ_k

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

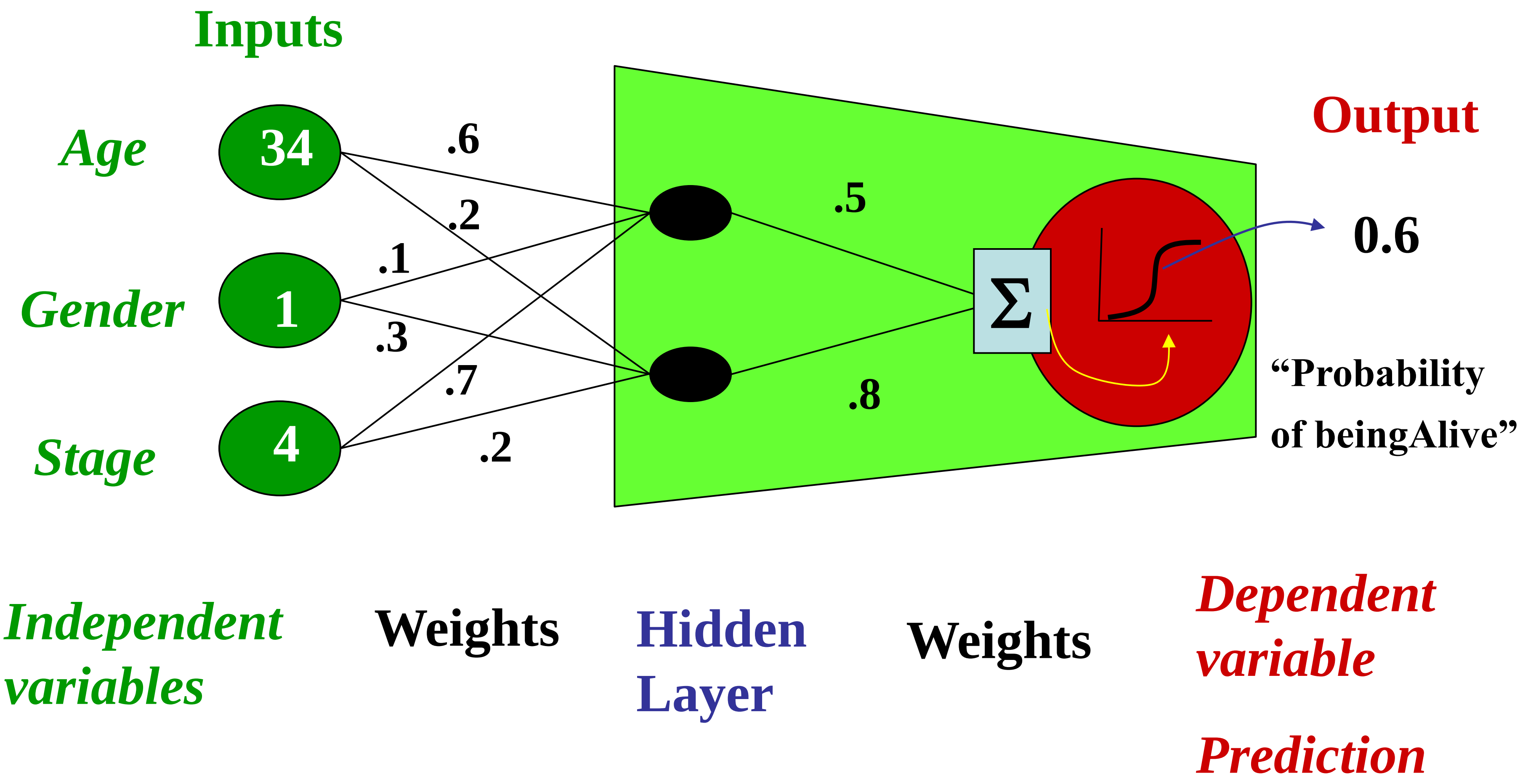
3. For each hidden unit h, calculate its error term δ_h

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

4. Update each network weight w_{ji}

$$w_{ji} \leftarrow w_{ji} + \eta \delta_k x_{ji}$$

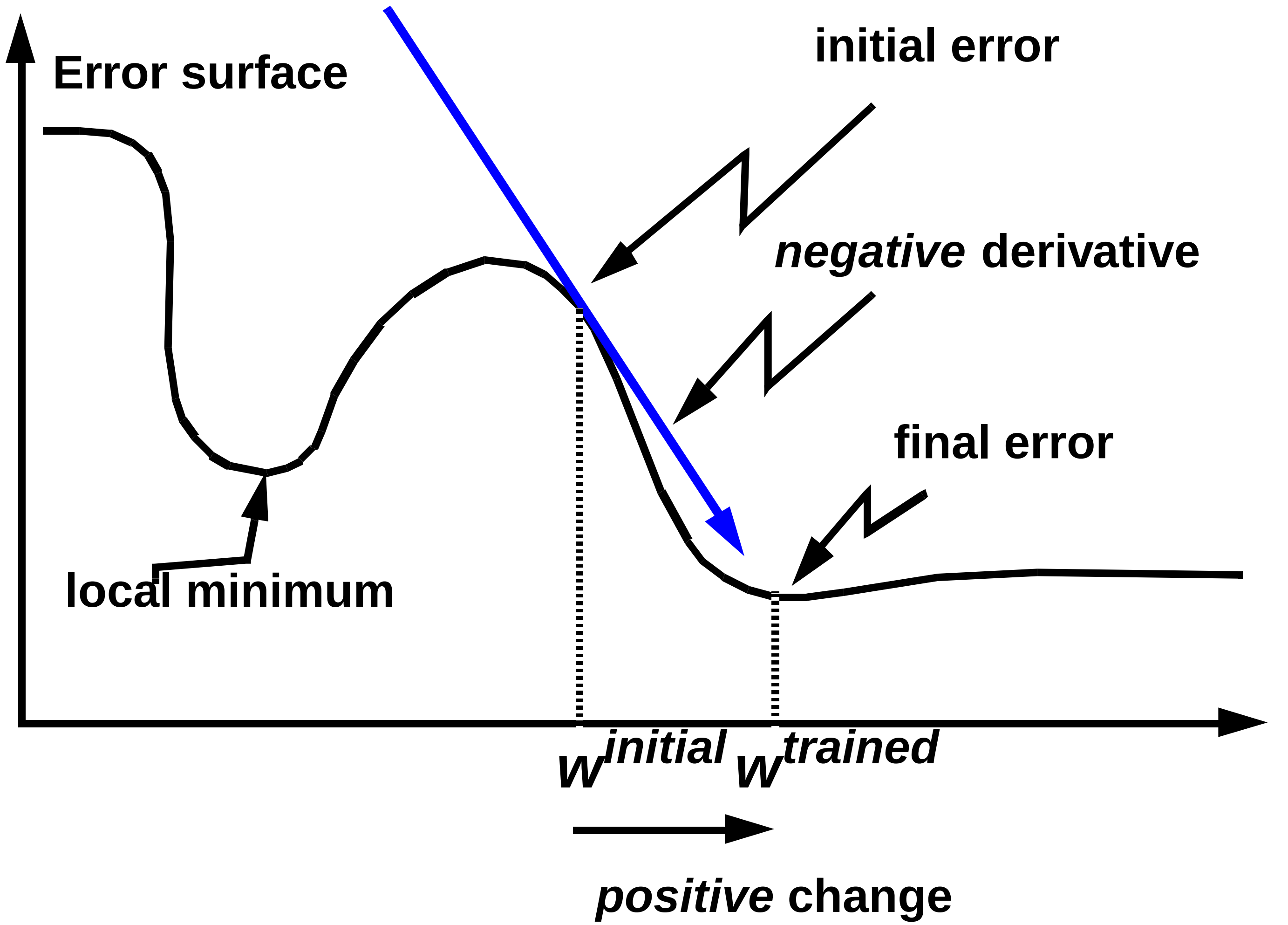
Learning Weights



The fine print

- Don’t implement back-propagation
  - Use a package
  - Better second-order or variable step-size optimization techniques exist
- Feature normalization
  - Typical to normalize inputs to lie in [0,1]
    - (and outputs must be normalized)
- Problems with NN training:
  - Slow training times
  - Local minima

Minimizing the Error

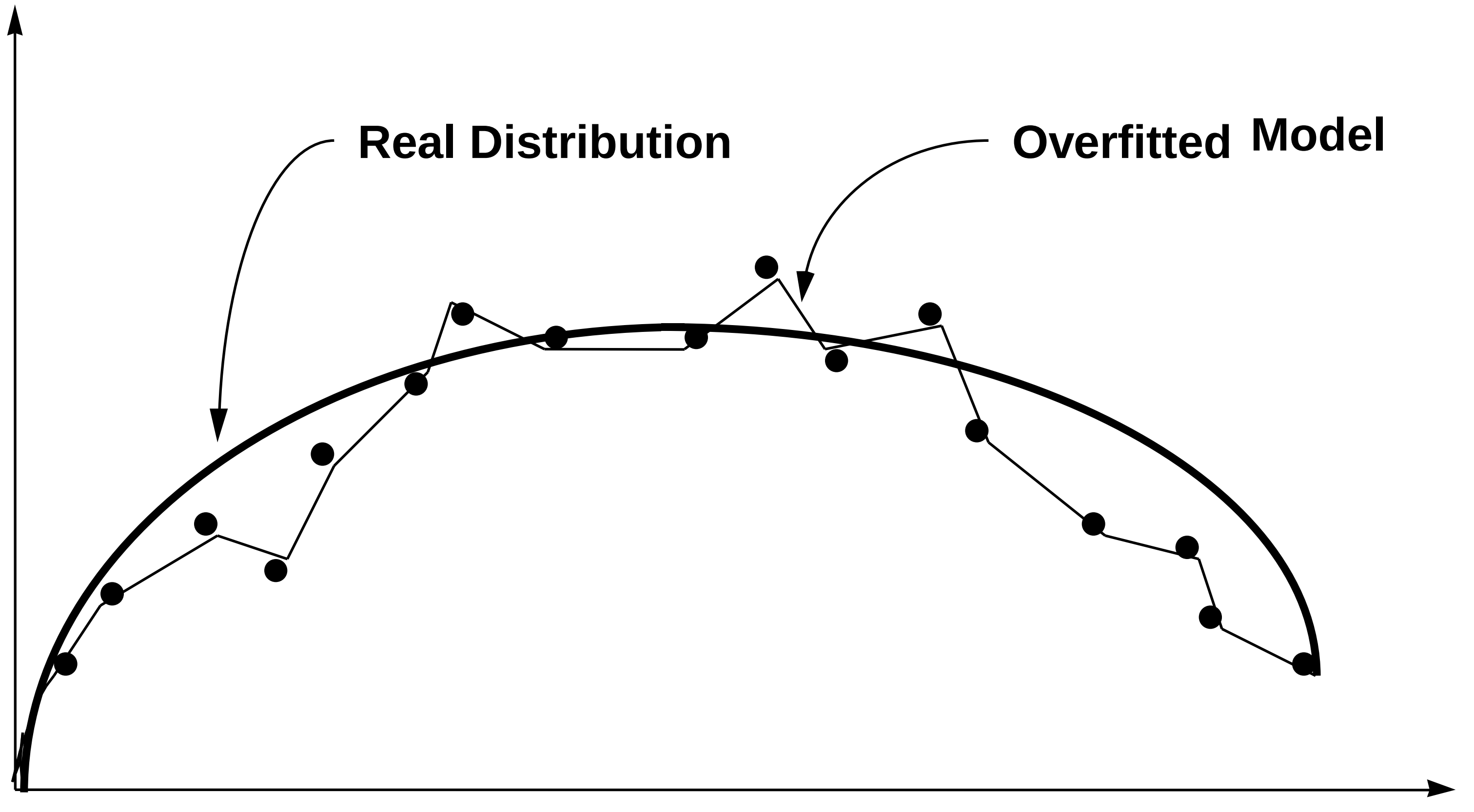


Expressive Power of ANNs

- Universal Function Approximator:
  - Given enough hidden units, can approximate *any* continuous function *f*
- Need 2+ hidden units to learn XOR

- Why not use millions of hidden units?
  - Efficiency (training is slow)
  - Overfitting

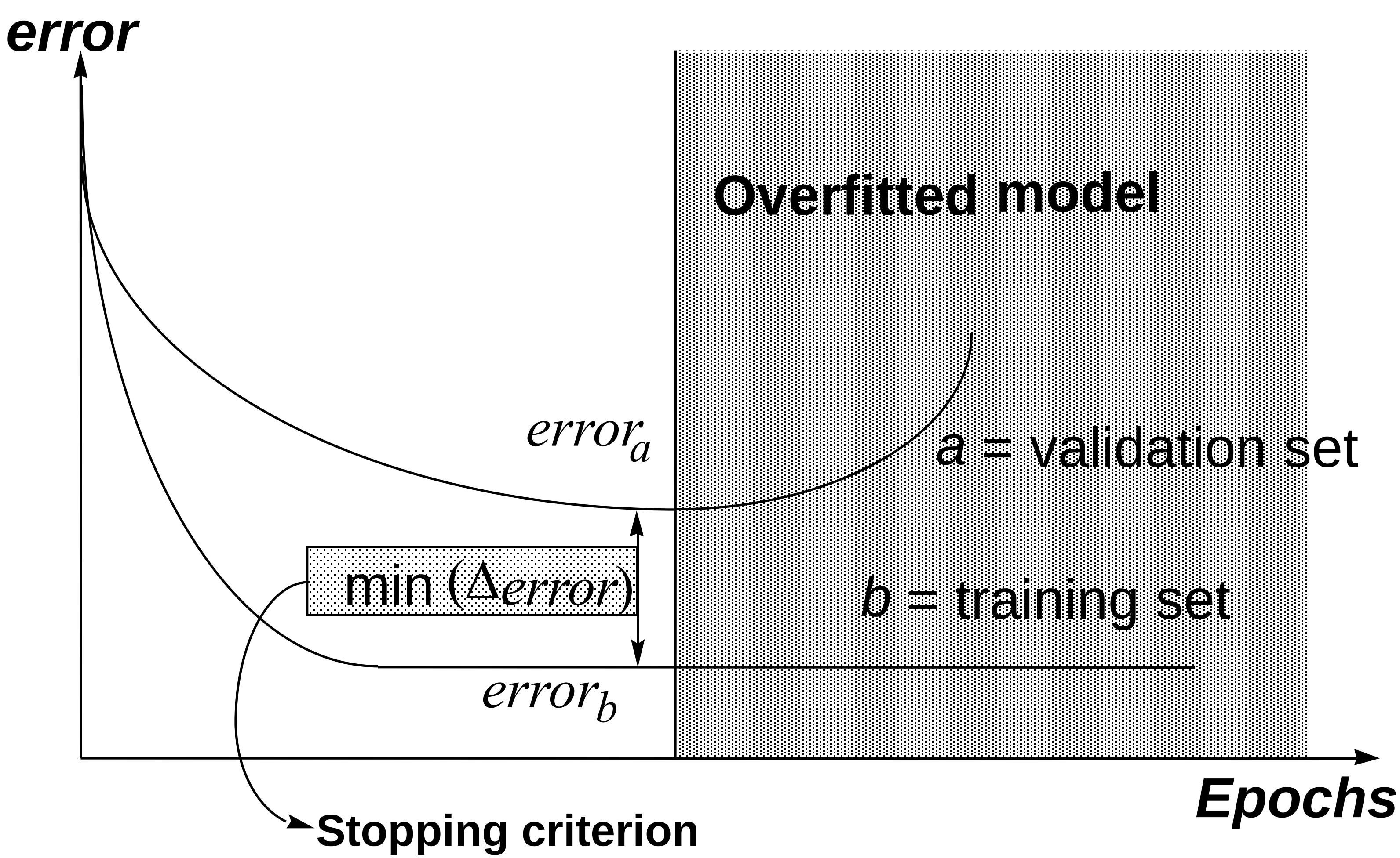
Overfitting



Combating Overfitting in Neural Nets

- Many techniques
- Two popular ones:
  - Early Stopping
    - Use “a lot” of hidden units
    - Just don’t over-train
  - Cross-validation
    - Test different architectures to choose “right” number of hidden units

Early Stopping



Cross-validation

- Cross-validation: general-purpose technique for model selection
  - E.g., “how many hidden units should I use?”
- More extensive version of validation-set approach.

Cross-validation

- Break training set into *k* sets
- For each model *M*
  - For *i*=1…*k*
    - Train *M* on all but set *i*
    - Test on set *i*
- Output *M* with highest average test score, trained on full training set

Summary of Neural Networks

When are Neural Networks useful?

- Instances represented by attribute-value pairs
  - Particularly when attributes are real valued
- The target function is
  - Discrete-valued
  - Real-valued
  - Vector-valued
- Training examples may contain errors
- Fast evaluation times are necessary

When not?

- Fast training times are necessary
- Understandability of the function is required

Summary of Neural Networks

Non-linear regression technique that is trained with gradient descent.

Question: How important is the biological metaphor?

Advanced Topics in Neural Nets

- Batch Move vs. incremental
- Hidden Layer Representations
- Hopfield Nets
- Neural Networks on Silicon
- Neural Network language models

Incremental vs. Batch Mode

Incremental mode Gradient Descent:
Do until satisfied

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

Batch mode Gradient Descent:
Do until satisfied

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

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

Incremental vs. Batch Mode

- In Batch Mode we minimize:

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

- Same as computing: $\Delta \vec{w}_D = \sum_{d \in D} \Delta \vec{w}_d$

- Then setting $\vec{w} \leftarrow \vec{w} + \Delta \vec{w}_D$

Advanced Topics in Neural Nets

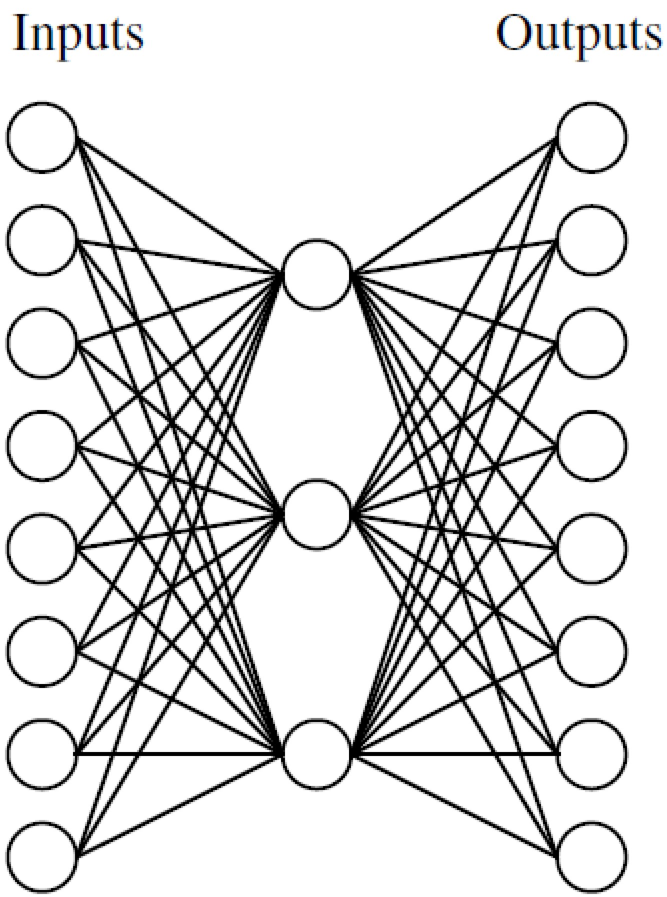
- Batch Move vs. incremental
- Hidden Layer Representations
- Hopfield Nets
- Neural Networks on Silicon
- Neural Network language models

Hidden Layer Representations

- Input->Hidden Layer mapping:
  - representation of input vectors tailored to the task
- Can also be exploited for *dimensionality reduction*
  - Form of unsupervised learning in which we output a "more compact" representation of input vectors
  - $\langle x_1, \ldots, x_n \rangle \rightarrow \langle x'_1, \ldots, x'_m \rangle$ where $m < n$
  - Useful for visualization, problem simplification, data compression, etc.

Dimensionality Reduction

Model:



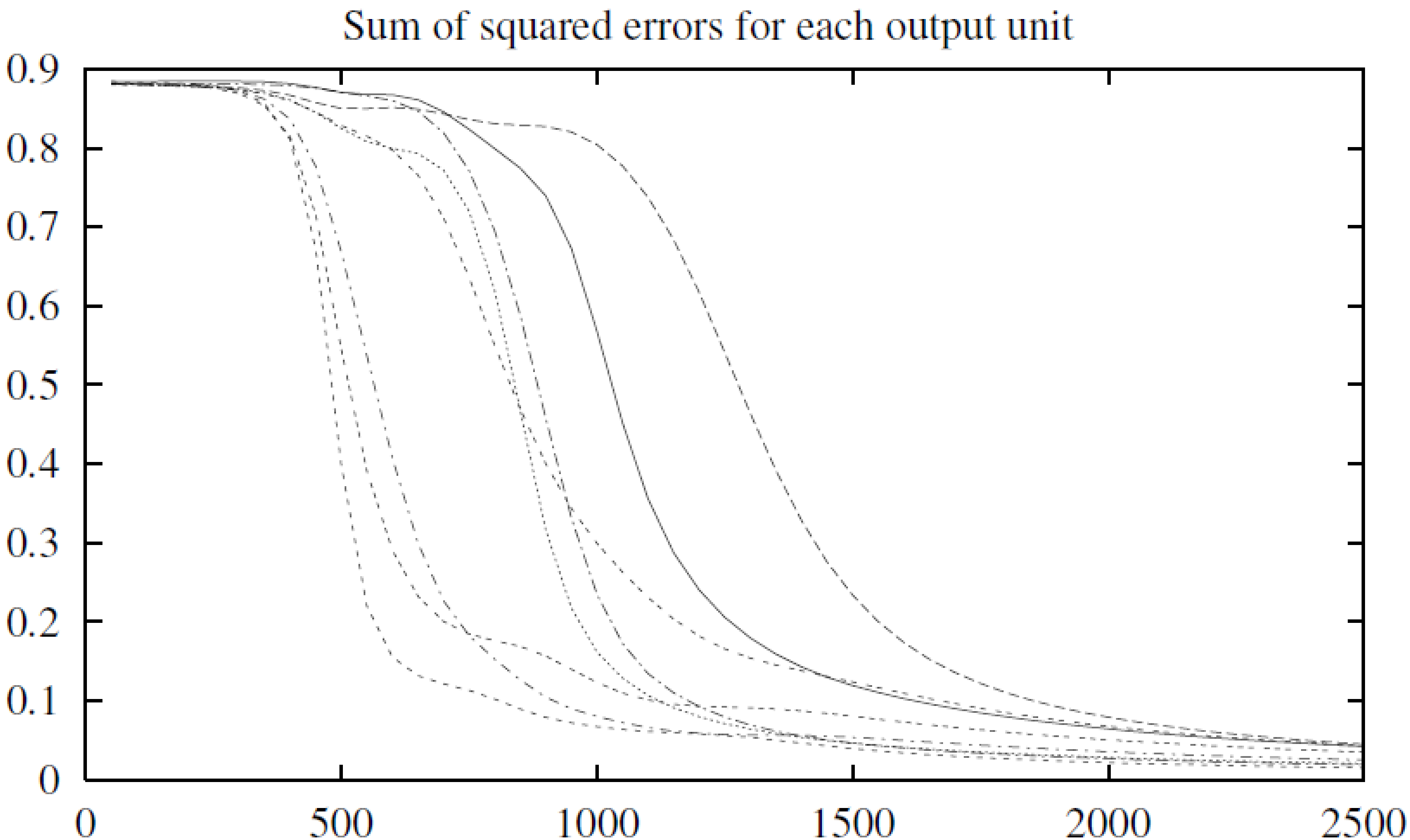
Function to learn:

Input		Output
10000000	$\rightarrow$	10000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	00000001

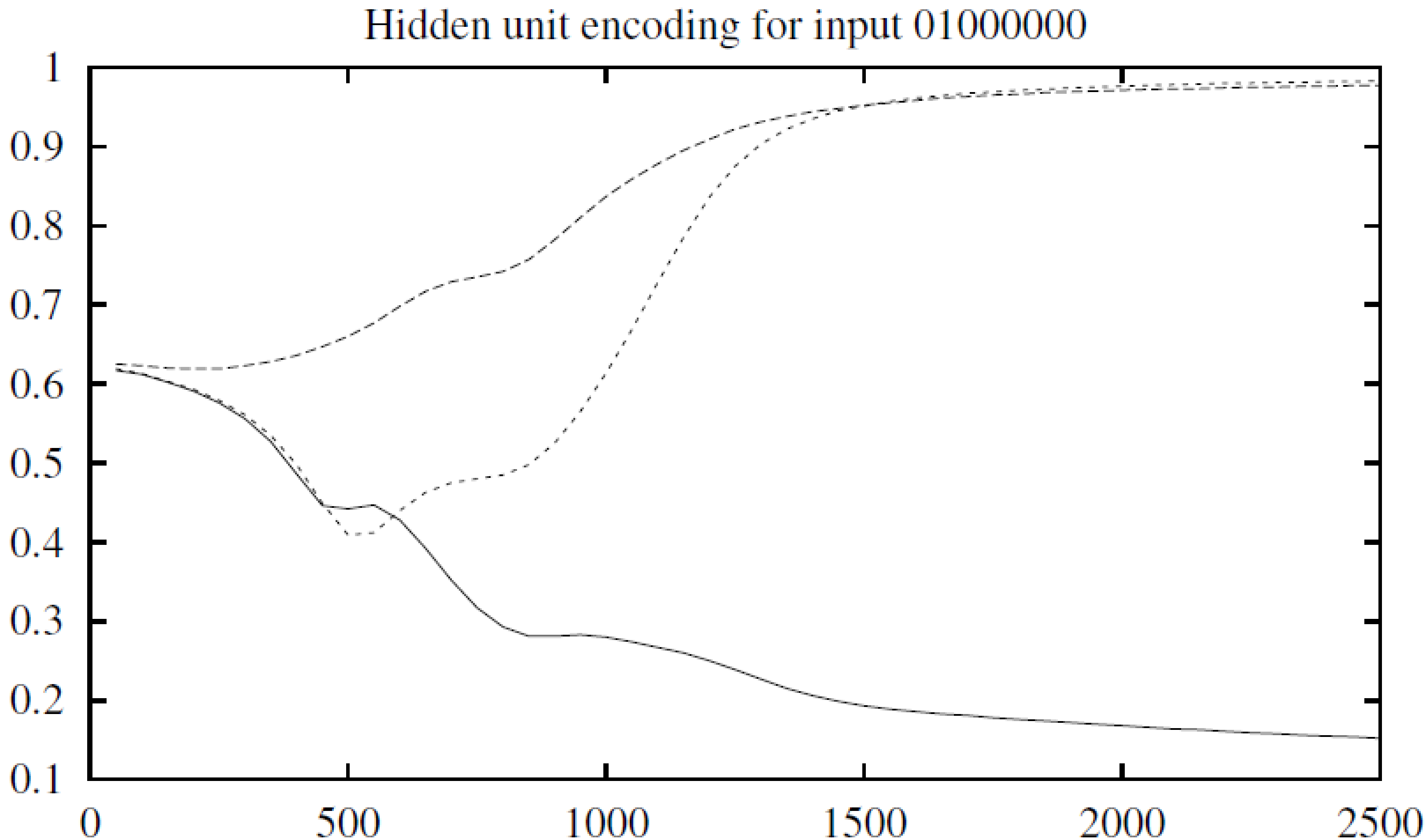
Dimensionality Reduction: Example

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

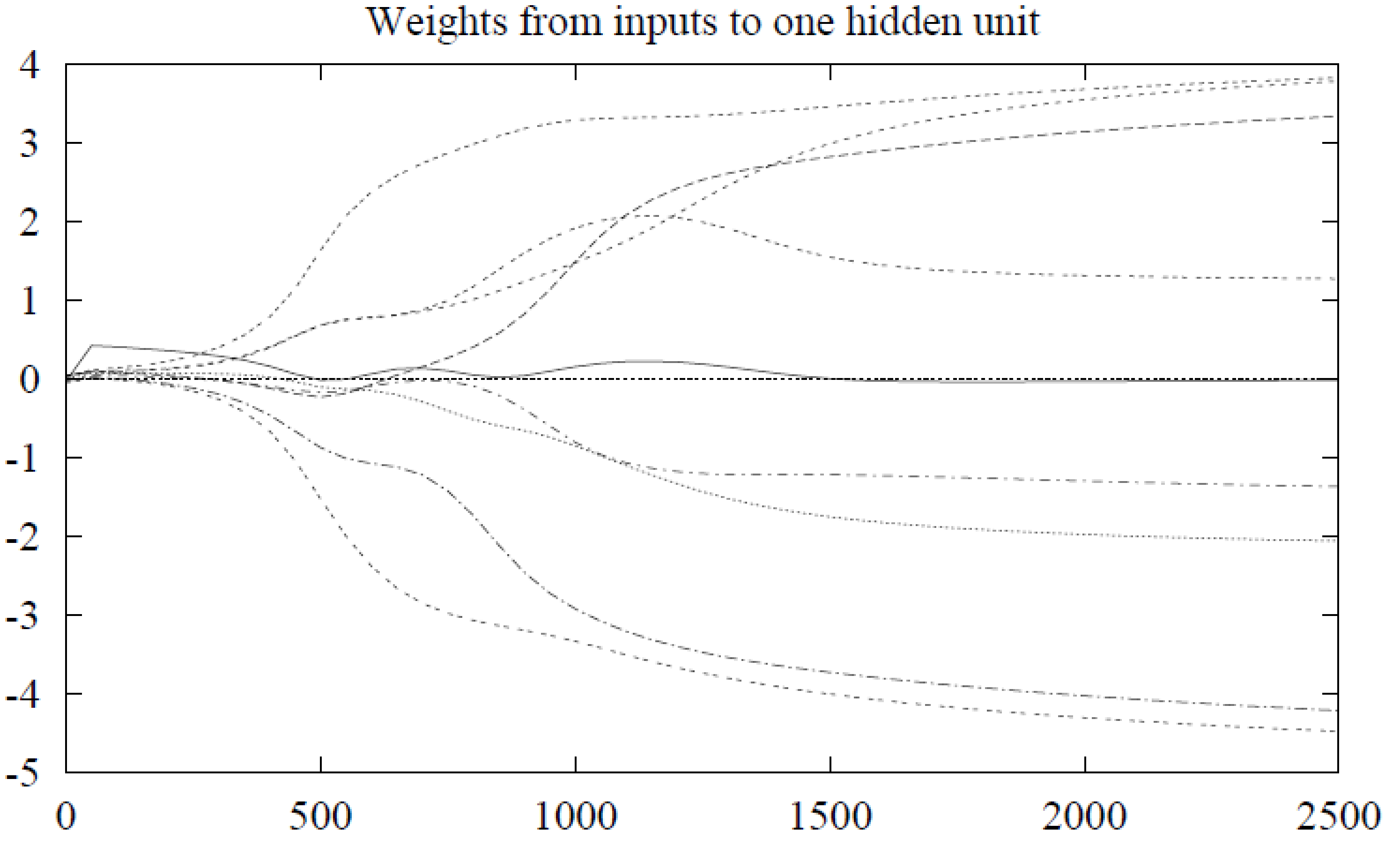
Dimensionality Reduction: Example



Dimensionality Reduction: Example



Dimensionality Reduction: Example



Advanced Topics in Neural Nets

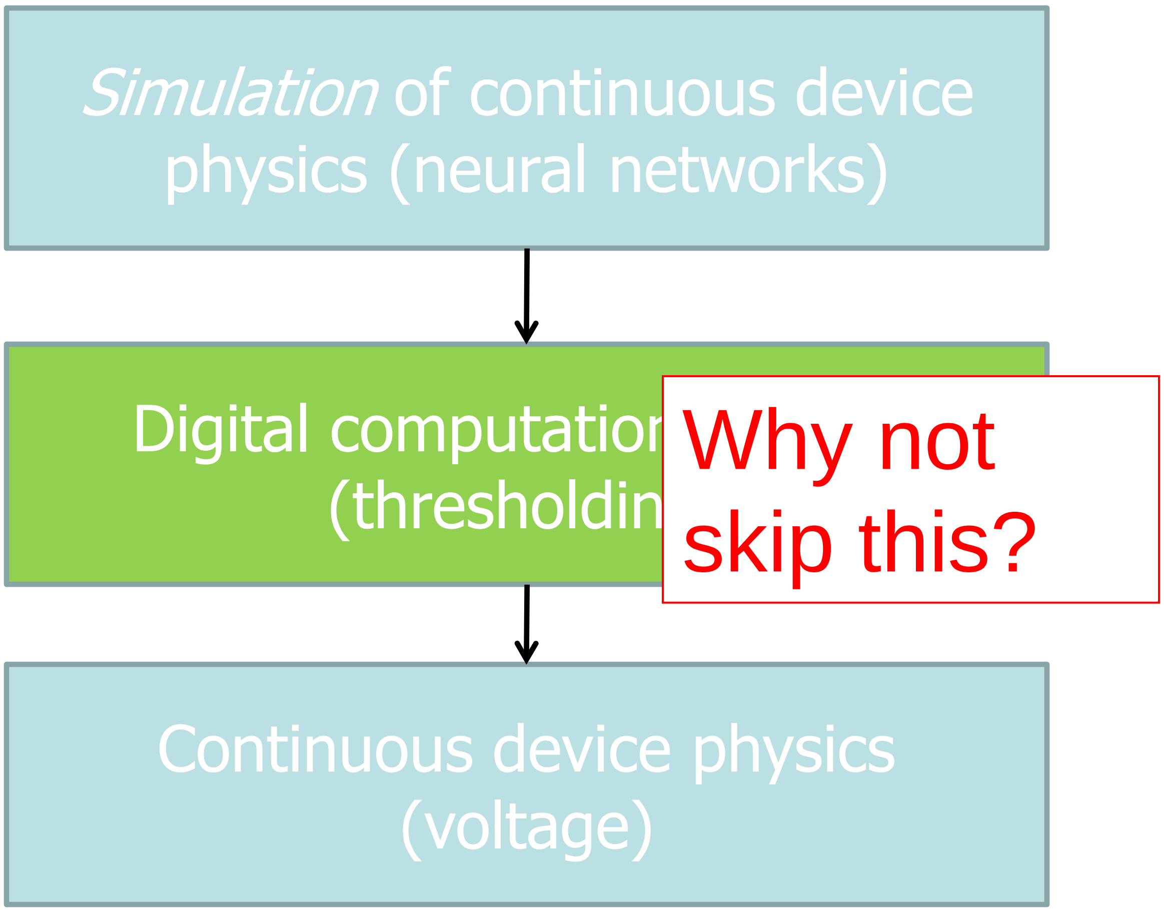
- Batch Move vs. incremental
- Hidden Layer Representations
- Hopfield Nets
- Neural Networks on Silicon
- Neural Network language models

Advanced Topics in Neural Nets

- Batch Move vs. incremental
- Hidden Layer Representations
- Hopfield Nets
- Neural Networks on Silicon
- Neural Network language models

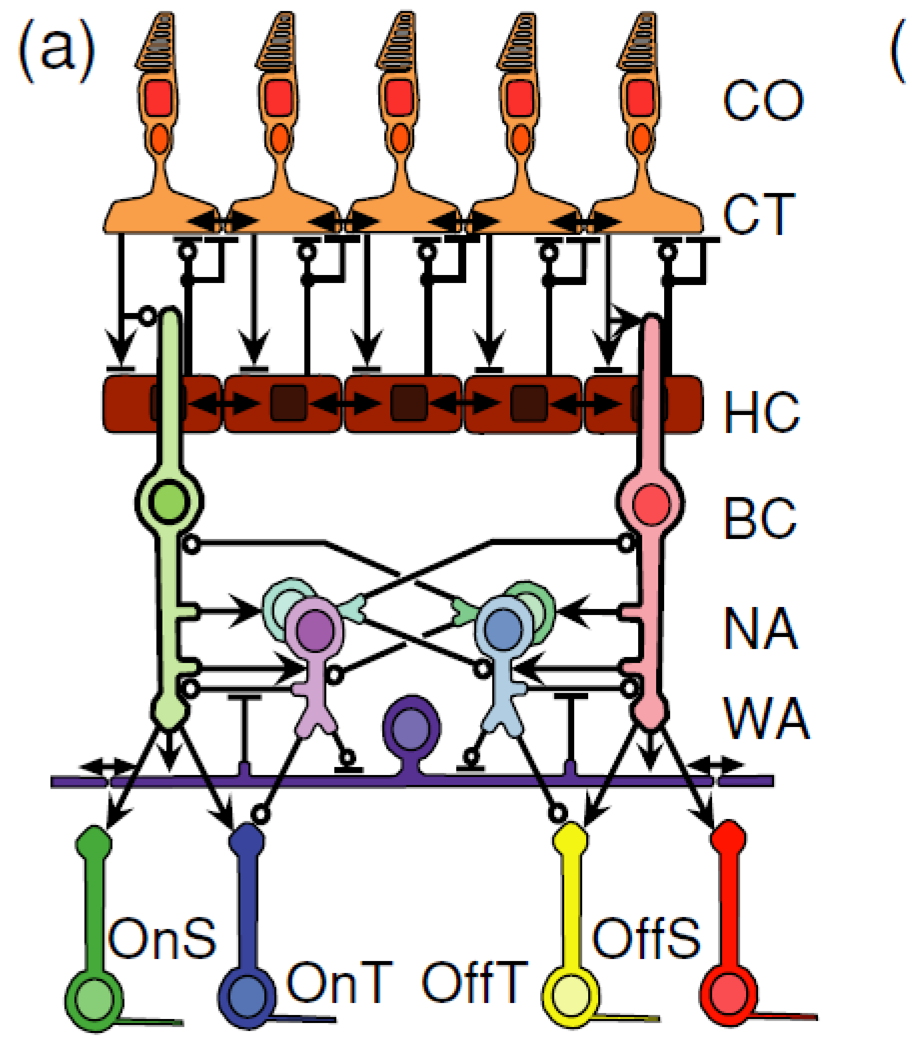
Neural Networks on Silicon

- Currently:



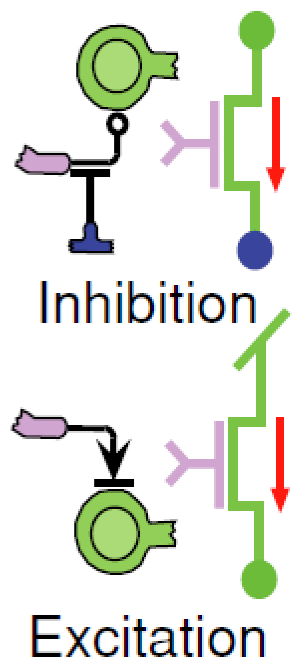
Example: Silicon Retina

- Simulates function of biological retina
- Single-transistor synapses adapt to luminance, temporal contrast
- Modeling retina directly on chip => requires 100x less power!

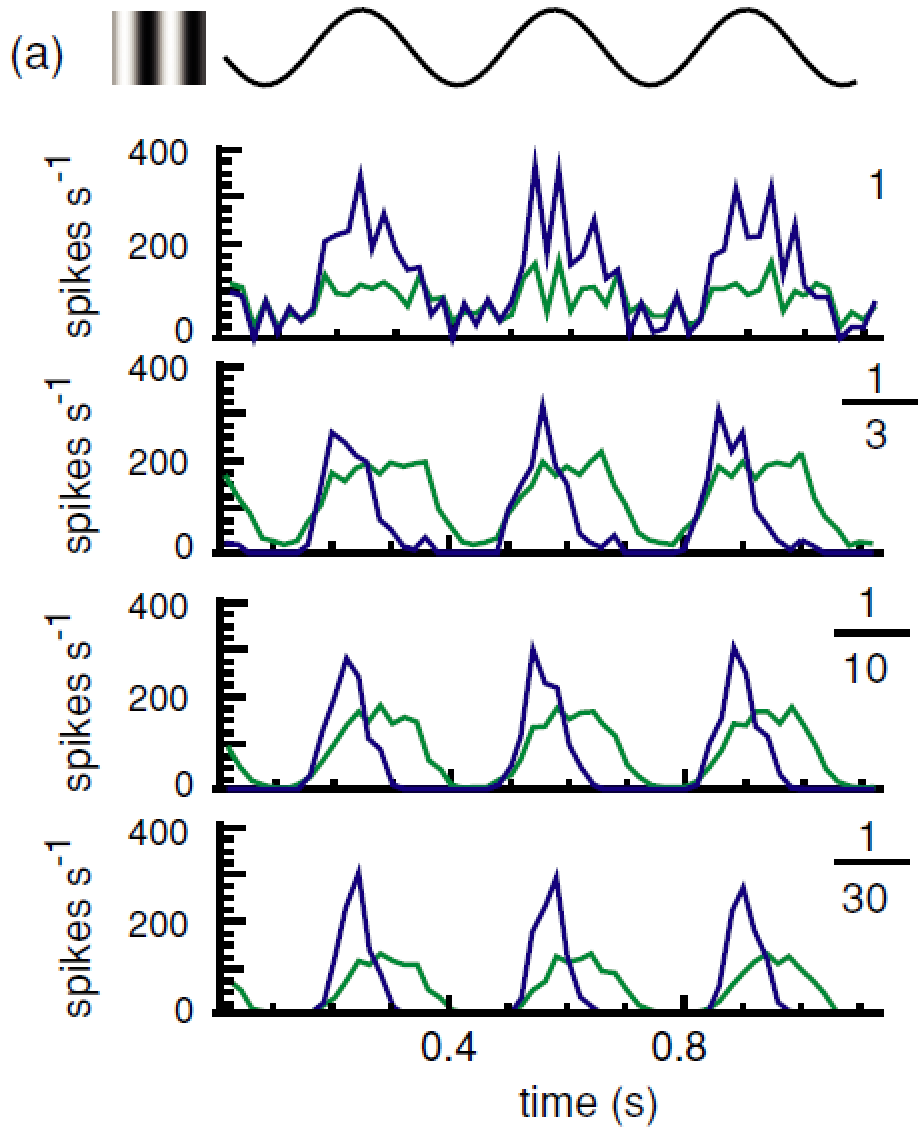


Example: Silicon Retina

- Synapses modeled with single transistors

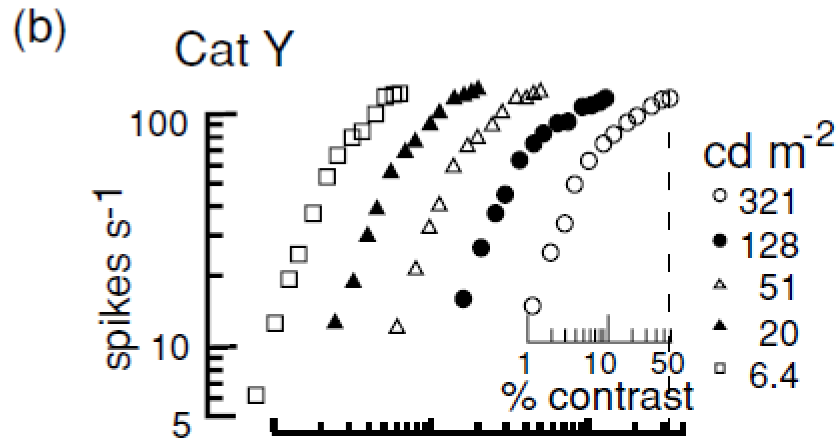


Luminance Adaptation

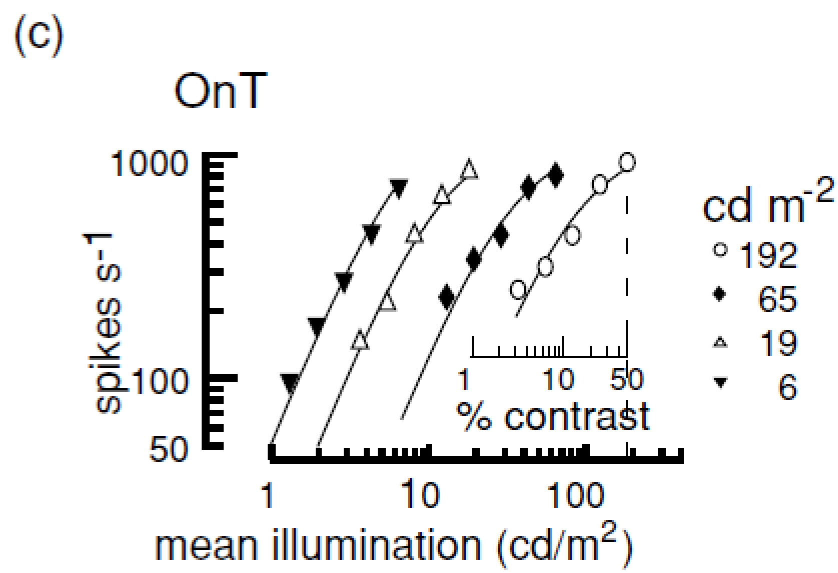


Comparison with Mammal Data

- Real:



- Artificial:



- Graphics and results taken from:

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF NEURAL ENGINEERING

J. Neural Eng. **3** (2006) 257–267 doi:10.1088/1741-2560/3/4/002

A silicon retina that reproduces signals in the optic nerve

Kareem A Zaghloul[1] and Kwabena Boahen[2,3]

General NN learning in silicon?

- *Seems* less in-vogue than in late 90s
- Interest has turned somewhat to implementing Bayesian techniques in analog silicon

Advanced Topics in Neural Nets

- Batch Move vs. incremental
- Hidden Layer Representations
- Hopfield Nets
- Neural Networks on Silicon
- Neural Network language models

Neural Network Language Models

- Statistical Language Modeling:
  - Predict probability of next word in sequence

`I was headed to Madrid , ____`

P(___ = "**`Spain`**") = 0.5,

P(___ = "**`but`**") = 0.2, etc.

- Used in speech recognition, machine translation, (recently) information extraction

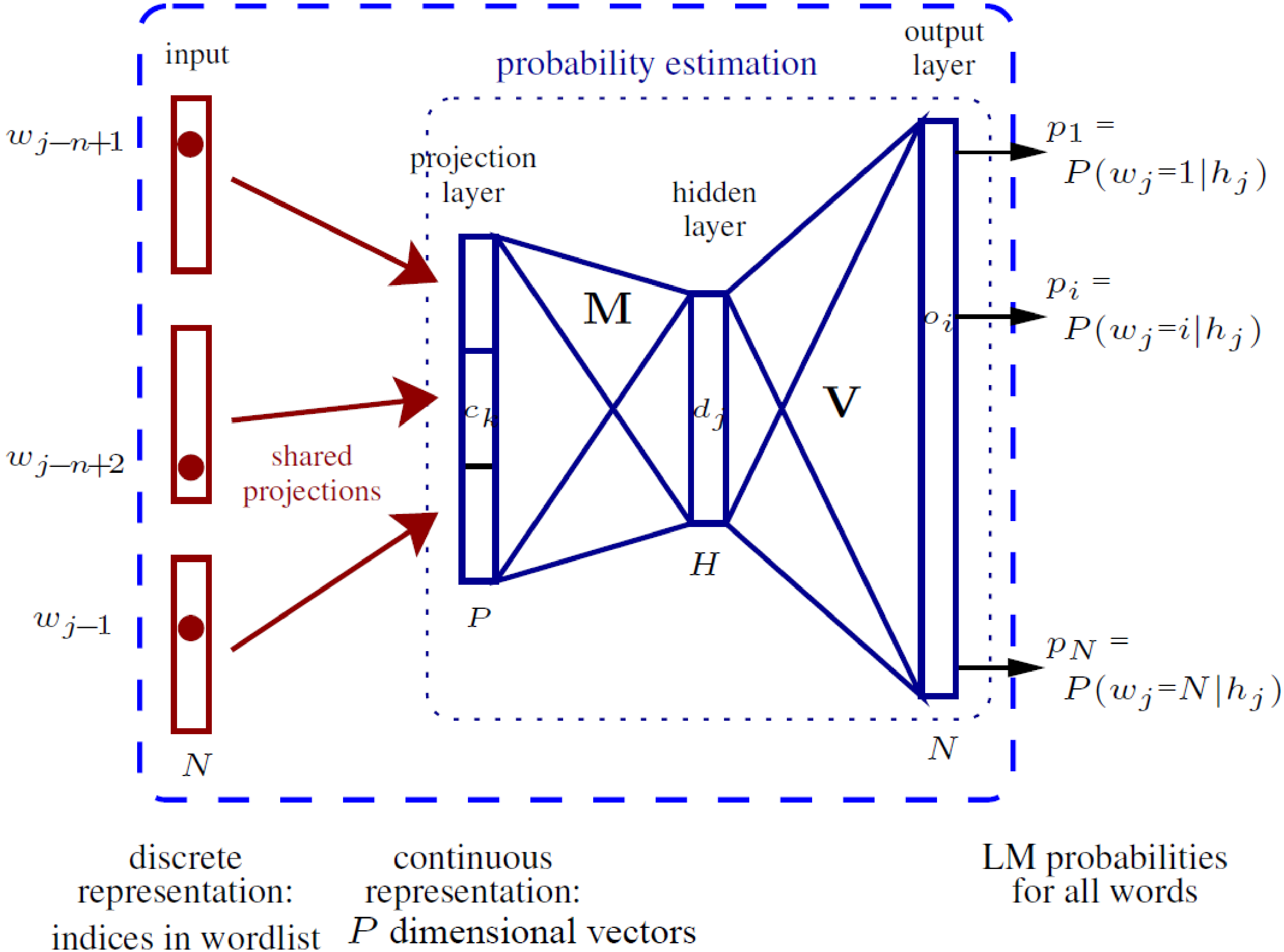
Formally

- Estimate:

$$P\left(w_j \mid w_{j-1}, w_{j-2}, \ldots, w_{j-n+1}\right)$$

$$= P\left(w_j \mid h_j\right)$$

Neural Network



Optimizations

- Key idea – learn simultaneously:
  - vector representations of each word (120 dim)
  - predictor of next word. based on previous vectors

- Short-lists
  - Much complexity in hidden->output layer
    - Number of possible next words is large
  - Only predict a *subset* of words
    - Use a standard probabilistic model for the rest

Design Decisions (1)

- Number of hidden units

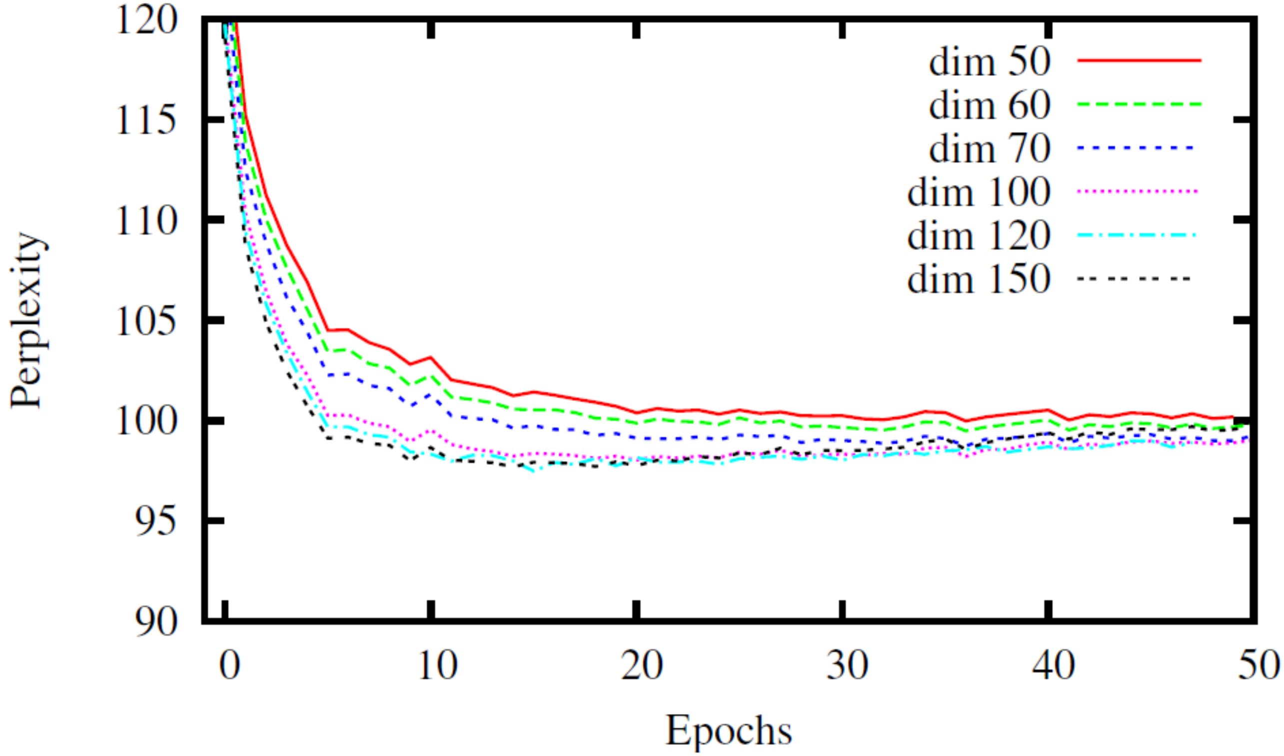
size	400	500	600	1000*
Tr. time	11h20	13h50	16h15	11+16h
Px alone	100.5	100.1	99.5	94.5
interpol.	68.3	68.3	68.2	68.0
Werr	13.99%	13.97%	13.96%	13.92%

* Interpolation of networks with 400 and 600 hidden units.

- Almost no difference…

Design Decisions (2)

- Word representation (# of dimensions)



- They chose 120

Comparison vs. state of the art

	Back-off LM	Neural Network LM				
Training data [#words]	600M	4M	22M	92.5M*	600M*	
Training time [h/epoch]	-	2h40	14h	9h40	12h	3×12h
Perplexity (NN LM alone)	-	103.0	97.5	84.0	80.0	76.5
Perplexity (interpolated LMs)	70.2	67.6	67.9	66.7	66.5	65.9
Word error rate (interpolated LMs)	**14.24%**	14.02%	13.88%	13.81%	**13.75%**	**13.61%**

* By resampling different random parts at the beginning of each epoch.