

Machine Learning: Part I

UMaine COS 470/570 – Introduction to AI
Spring 2019

Machine Learning:
Part I

Introduction
Perceptrons
Nonlinear neurons
Feedforward
neural networks
Matrix form of NN
Gradient descent
learning in FFNs
Backpropagation
Deep learning
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What are ANNs?

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Artificial neural networks

- ▶ Systems of simple computing elements: *neurons*
- ▶ Each neuron accepts inputs from others, produces *activation*
- ▶ Neurons connected via *weights* that modulate activation
- ▶ Can be viewed as:
 - ▶ Pattern-learning (inductive) systems
 - ▶ Statistical programs
 - ▶ Dimension/feature-changing systems
 - ▶ Search programs (in weight space)

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What can they do?

- ▶ Image classification and labeling
- ▶ Word recognition
- ▶ Natural language systems
- ▶ Machine translation systems
- ▶ General pattern recognition
- ▶ Superhuman-level performance on games, other RL tasks
- ▶ Pattern generators (images, music, ...)

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Inspiration: Natural pattern recognition

- ▶ Pattern recognition in natural world:
 - ▶ Chemoreceptors
 - ▶ Immune system
 - ▶ Biological neural networks
 - ▶ Animal/human vision system
 - ▶ Auditory system
 - ▶ Neocortex
 - ▶ Etc.

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Neural systems

- ▶ Most flexible pattern recognizers:
- ▶ Biological computing elements: Neurons
- ▶ Neurons are *excitatory* cells
- ▶ Connections determine how activation spreads

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Problem: Complexity

- ▶ Neurons are *very* complex

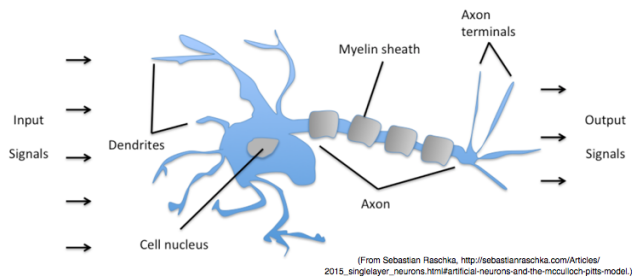
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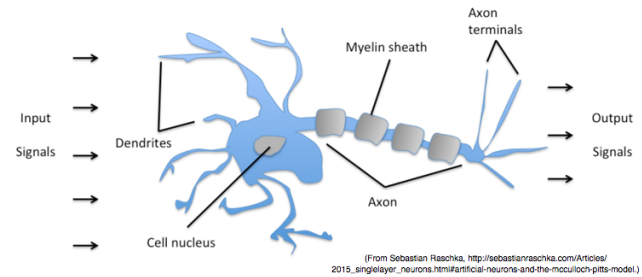
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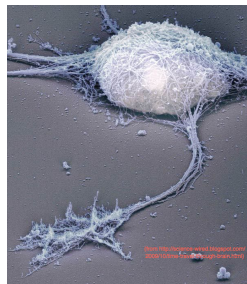
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- ▶ Synapses: change potential across cell membrane
- ▶ Neuron effectively sums excitations, inhibitions
- ▶ At some point: potential at threshold and neuron *fires*
- ▶ Excitatory pulse down axon, release neurotransmitter at synapses
- ▶ *Lots* more to it than this!

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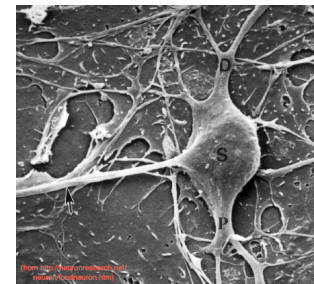
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Problem: Complexity

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- ▶ Connectsome is incredibly complex

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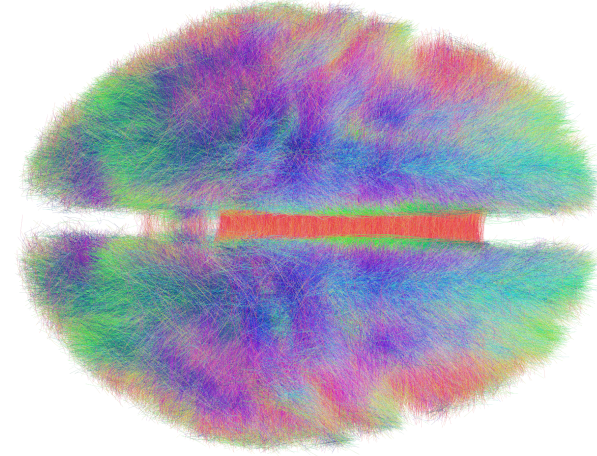


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First simple artificial neuron: Perceptron

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- ▶ McCulloch & Pitts
- ▶ **Very** simple model of a neuron

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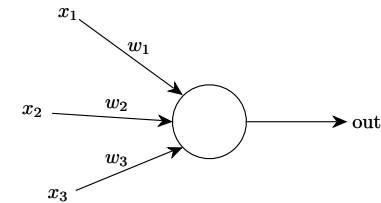
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First simple artificial neuron: Perceptron

Machine Learning:
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- ▶ McCulloch & Pitts
- ▶ **Very** simple model of a neuron



$$\text{output} = \begin{cases} 0 & \text{if } \sum_j w_j x_j \leq \text{threshold} \\ 1 & \text{otherwise} \end{cases}$$

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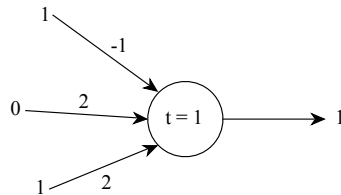
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First simple artificial neuron: Perceptron

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First simple artificial neuron: Perceptron

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- ▶ McCulloch & Pitts
- ▶ **Very** simple model of a neuron
- ▶ Usually change threshold to **bias** (= -threshold)

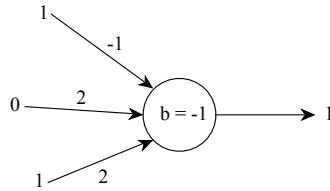
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First simple artificial neuron: Perceptron

- ▶ McCulloch & Pitts
- ▶ *Very* simple model of a neuron
- ▶ Usually change threshold to *bias* (= -threshold)



$$\text{output} = \begin{cases} 0 & \text{if } \sum_j w_j x_j + b \leq 0 \\ 1 & \text{otherwise} \end{cases}$$

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What can they do?

- ▶ “Weigh evidence” \Rightarrow decision

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What can they do?

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- ▶ E.g.:

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What can they do?

- ▶ “Weigh evidence” \Rightarrow decision
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What can they do?

- ▶ “Weigh evidence” \Rightarrow decision
- ▶ E.g.:
 - ▶ output = “study”
 - ▶ x_1 = test on Monday, x_2 = confident of material, x_3 = doing poorly in class
 - ▶ $w_1 = 1$, $w_2 = -1$, $w_3 = 2$
 - ▶ bias = 0
 - ▶ Test on Monday, confident, doing well in class \Rightarrow output = 0
 - ▶ Test on Monday, not confident, doing well \Rightarrow output = 1

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 - ▶ bias = 0
 - ▶ Test on Monday, confident, doing well in class \Rightarrow output = 0
 - ▶ Test on Monday, not confident, doing well \Rightarrow output = 1
 - ▶ Test on Monday, confident, doing poorly:
 $1 + (-1) + 2 = 2 \Rightarrow$ output = 1

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Learning the weights

- ▶ Rosenblatt’s perceptron algorithm

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Learning the weights

- ▶ Rosenblatt’s perceptron algorithm
- ▶ Use *training examples*

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Learning the weights

- ▶ Rosenblatt's perceptron algorithm
- ▶ Use *training examples*
- ▶ Modify weights such that output error is minimized

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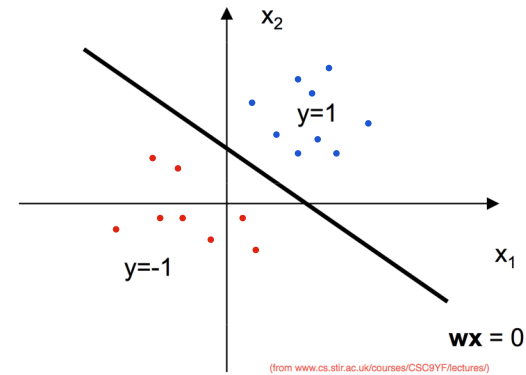
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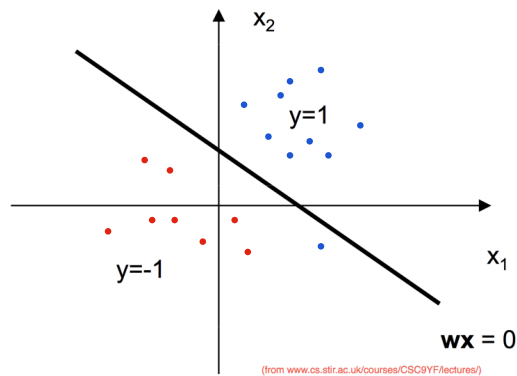
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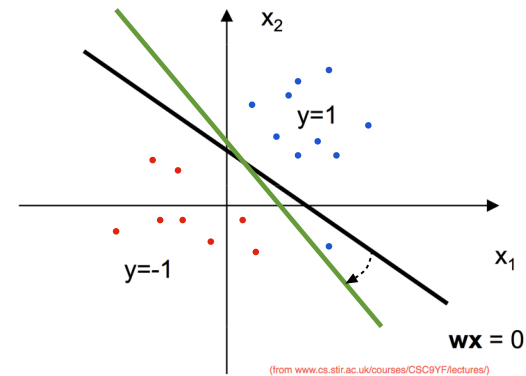
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- ▶ Let:
 - ▶ y_k = desired output for example k
 - ▶ a_k = actual output for example k
- ▶ Error on example $k = y_k - a_k$
- ▶ Define an error function E_k for example k

$$E = \sum_k E_k = \frac{1}{2} \sum_k (y_k - a_k)^2$$

- ▶ Why?
 - ▶ Squaring make error always positive (parabola)
 - ▶ The 1/2 “makes the math easier” (as we’ll see)

Learning the weights

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- ▶ Goal: minimize E by minimizing each E_k

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- ▶ Goal: minimize E by minimizing each E_k
- ▶ E_k is a function of the weights

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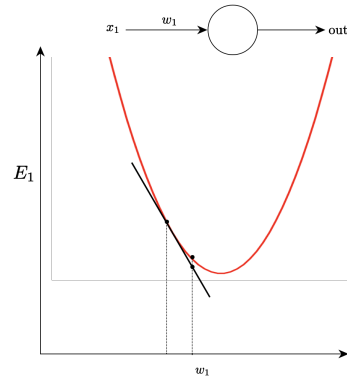
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- ▶ Goal: minimize E by minimizing each E_k
- ▶ E_k is a function of the weights
- ▶ Use *gradient descent* instead

Learning the weights

- ▶ Goal: minimize E by minimizing each E_k
- ▶ E_k is a function of the weights
- ▶ Use *gradient descent* instead
- ▶ With one weight:



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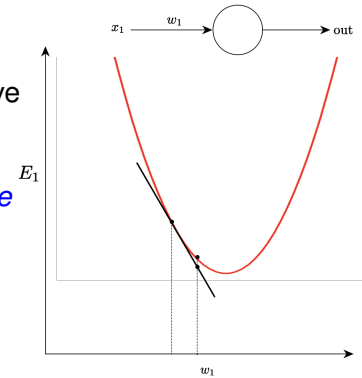
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Learning the weights

- ▶ Goal: minimize E by minimizing each E_k
- ▶ E_k is a function of the weights
- ▶ Use *gradient descent* instead
- ▶ With one weight:
- ▶ Slope at point: $\frac{dE_k}{dx_i}$
tells which direction to move
 $w'_1 = w_1 - \alpha \frac{dE_k}{dx_i}$
where α is the *learning rate*



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Learning the weights

- ▶ Suppose there are 2 weights, x and y

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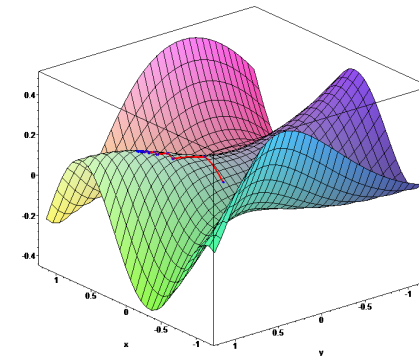
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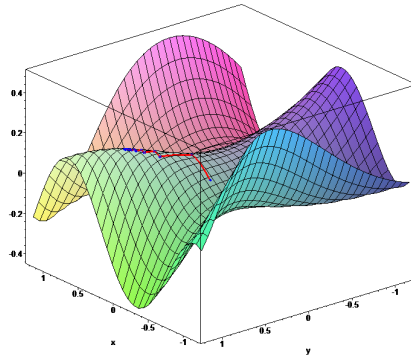
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- Suppose there are 2 weights, x and y



- Now “slope” is really the **gradient** ∇ at (x, y)

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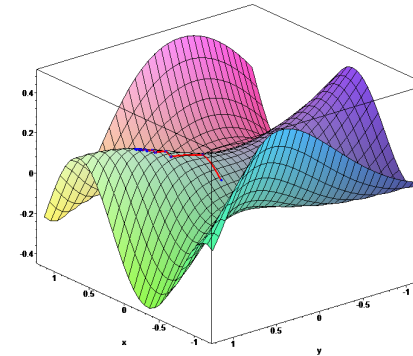
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Learning the weights

- Suppose there are 2 weights, x and y



- Now “slope” is really the **gradient** ∇ at (x, y)

$$\nabla(w_i) = \frac{\partial E_k}{\partial w_i} \text{ and } w_{i,t+1} = w_{i,t} - \alpha \frac{\partial E_k}{\partial w_{i,t}}$$

- Gradient descent: hill-climbing in multiple dimensions

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Learning the weights

- What is $\frac{\partial E_k}{\partial w_i}$?

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Learning the weights

- What is $\frac{\partial E_k}{\partial w_i}$?
- We know that the output for k^{th} example $a_k = \sum_i w_i x_i$

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Learning the weights

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- ▶ What is $\frac{\partial E_k}{\partial w_i}$?
- ▶ We know that the output for k^{th} example $a_k = \sum_i w_i x_i$
- ▶ **Chain rule:**

$$\begin{aligned}\frac{\partial E_k}{\partial w_i} &= \frac{\partial E_k}{\partial a_k} \frac{\partial a_k}{\partial w_i} \\ &= \frac{\partial \frac{1}{2}(y_k - a_k)^2}{\partial a_k} \frac{\partial (w_1 x_1 + w_2 x_2 + \dots w_n x_n)}{\partial w_i} \\ &= -(y_k - a_k) x_i\end{aligned}$$

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- ▶ We know that the output for k^{th} example $a_k = \sum_i w_i x_i$
- ▶ **Chain rule:**

$$\begin{aligned}\frac{\partial E_k}{\partial w_i} &= \frac{\partial E_k}{\partial a_k} \frac{\partial a_k}{\partial w_i} \\ &= \frac{\partial \frac{1}{2}(y_k - a_k)^2}{\partial a_k} \frac{\partial (w_1 x_1 + w_2 x_2 + \dots w_n x_n)}{\partial w_i} \\ &= -(y_k - a_k) x_i\end{aligned}$$

- ▶ Since $\Delta w_i = \alpha \frac{\partial E_k}{\partial w_i}$, then

$$w_{i,t+1} = w_{i,t} - \alpha(-(y_k - a_k) x_i) = w_{i,t} + \alpha(y_k - a_k) x_i$$

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- ▶ So for each example $\langle (x_1, x_2, \dots, x_n), y \rangle$
 - ▶ Compute output a
 - ▶ Adjust weights:

$$w_{i,t+1} = w_{i,t} + \alpha(y - a)x_i$$

for all weights w_i

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- ▶ Algorithm first in IBM 704 in late 50s

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Implementations

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- ▶ Then:

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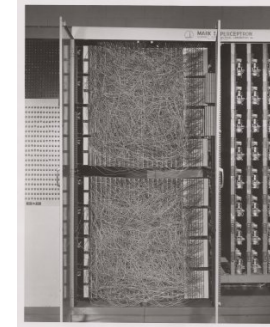
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Implementations

- ▶ Algorithm first in IBM 704 in late 50s
- ▶ Then:



- ▶ Mark I Perceptron Machine (Wikipedia)

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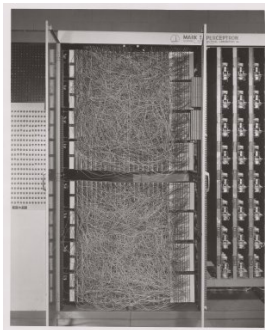
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Implementations

- ▶ Algorithm first in IBM 704 in late 50s
- ▶ Then:



- ▶ Mark I Perceptron Machine (Wikipedia)
- ▶ Image recognition: 20×20 photocell array
- ▶ Potentiometers: weights
- ▶ Pots adjusted by motors from learning

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Example

```
(defclass perceptron ()
  ((num-inputs :initarg :num-inputs :initform 3
               :accessor num-inputs)
   (inputs :initarg :inputs :initform nil :accessor inputs)
   (weights :initarg :weights :initform nil
            :accessor weights)
   (bias :initarg :bias :initform 0 :accessor bias)
   (output :initarg :output :initform nil :accessor output)
   (target :initarg :target :initform nil :accessor target)
   (alpha :initarg :alpha :initform 1.0 :accessor alpha)
  )

  (defmethod initialize-instance :after ((self perceptron)
                                         &rest l)

    (declare (ignore l))
    (with-slots (num-inputs weights) self
      (setq weights
        (loop for i from 1 to num-inputs
              collect (random 1.0)))))
```

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```
(defmethod compute-output ((self perceptron))
  (with-slots (output bias inputs weights) self
    (setq output (if (> (+ bias
                          (apply #'(+
                                (mapcar #'* inputs
                                      weights)))
                        0.0)
                    1
                    0))))

(defmethod adjust-weights ((self perceptron))
  (with-slots (inputs weights target output alpha) self
    (compute-output self)
    (let ((delta (loop for weight in weights
                        for input in inputs
                        collect (* alpha (- target output)
                                         input)))))
      (format t
        "~s -> ~s (desired = ~s), weights=~s, delta=~s~%"
        inputs output target weights delta)
      (setq weights (mapcar #'(+ weights delta)))
      (format t "      new weights=~s~%" weights))))
```

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```
(defmethod train ((self perceptron) examples)
  (with-slots (inputs target output weights) self
    (loop for count from 1 to (length examples)
          for example in examples
          do (setf inputs (car example)
                    target (cadr example))
              (compute-output self)
              (adjust-weights self)
              (compute-output self)
              )))
```

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```
(defvar *perceptron* nil)

(defun train-for-tt (&key new? examples (bias -6) (inputs 3))
  (when new?
    (setq *perceptron* (make-instance 'perceptron
                                       :bias bias :num-inputs inputs)))
  (train *perceptron* examples)
  ;; now check it:
  (loop for thing in examples
        do (setf (inputs *perceptron*) (car thing))
            (compute-output *perceptron*)
            (format t "~s => ~s~%" (car thing)
                                  (output *perceptron*))))
```

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```
(defvar *and-tt* '(((0 0) 0)
                  ((0 1) 0)
                  ((1 0) 0)
                  ((1 1) 1)))

(defvar *or-tt* '(((0 0) 0)
                  ((0 1) 1)
                  ((1 0) 1)
                  ((1 1) 1)))

(defvar *xor-tt* '(((0 0) 0)
                  ((0 1) 1)
                  ((1 0) 1)
                  ((1 1) 0)))
```

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What can it do?

- ▶ **Linear classifier:**
 - ▶ Finds line/plane/hyperplane separating class 1 from class 2
 - ▶ 2 inputs \Rightarrow line between sets
 - ▶ 3 inputs \Rightarrow plane, etc.
 - ▶ Sets can be separated by hyperplane \Rightarrow *linearly-separable*
- ▶ Training set linearly-separable, algorithm converges
- ▶ Example: can learn NAND function

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What can it do?

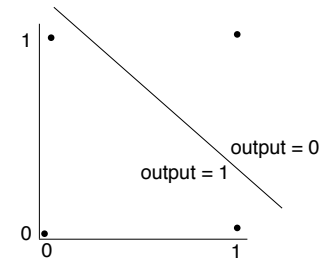
- ▶ **Linear classifier:**
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Problems

- ▶ May not be a unique solution

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Problems

- ▶ May not be a unique solution
 - ▶ Thus may have suboptimal learning
 - ▶ **Support vector machine (SM):** “perceptron of optimal stability”

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Extending perceptrons

Perceptron networks

- ▶ Single perceptron: very limited

Perceptron networks

- ▶ Single perceptron: very limited
- ▶ Idea: hook a bunch together in a network

Perceptron networks

- ▶ Single perceptron: very limited
- ▶ Idea: hook a bunch together in a network
- ▶ What can a perceptron network do?

Perceptron networks

Machine Learning:
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- ▶ Single perceptron: very limited
- ▶ Idea: hook a bunch together in a network
- ▶ What can a perceptron network do?
 - ▶ Based on what you know, what do *you* think?

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- ▶ What can a perceptron network do?
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 - ▶ Hint: perceptron can implement NAND function

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 - ▶ NAND forms complete gate/boolean function set

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 - ▶ $\therefore \Rightarrow$ any binary function, \Rightarrow Turing-equivalent

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 - ▶ NAND forms complete gate/boolean function set
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- ▶ E.g., a half-adder

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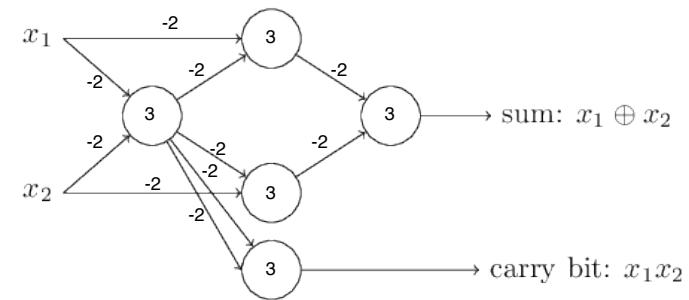
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Perceptron networks

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- ▶ Single perceptron: very limited
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- ▶ What can a perceptron network do?
 - ▶ Based on what you know, what do *you* think?
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 - ▶ NAND forms complete gate/boolean function set
 - ▶ $\therefore \Rightarrow$ any binary function, \Rightarrow Turing-equivalent
- ▶ E.g., a half-adder:



Cc

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Learning

Machine Learning:
Part I

- ▶ So we're done, right?

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Machine Learning:
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- ▶ So we're done, right?
- ▶ Not quite

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Machine Learning:
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- ▶ So we're done, right?
- ▶ Not quite
- ▶ Want property: small $\Delta w \Rightarrow$ small Δoutput

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Machine Learning:
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- ▶ So we're done, right?
- ▶ Not quite
- ▶ Want property: small $\Delta w \Rightarrow$ small Δoutput
- ▶ But perceptrons have *step function*

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Machine Learning:
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- ▶ So we're done, right?
- ▶ Not quite
- ▶ Want property: small $\Delta w \Rightarrow$ small Δoutput
- ▶ But perceptrons have *step function*
- ▶ Small input change can give completely different output

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- ▶ Not quite
- ▶ Want property: small $\Delta w \Rightarrow$ small Δoutput
- ▶ But perceptrons have *step function*
- ▶ Small input change can give completely different output
- ▶ Step function isn't *differentiable*

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- ▶ So we're done, right?
- ▶ Not quite
- ▶ Want property: small $\Delta w \Rightarrow$ small Δoutput
- ▶ But perceptrons have *step function*
- ▶ Small input change can give completely different output
- ▶ Step function isn't *differentiable*
- ▶ Can't easily find weights \Rightarrow minimum error

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Nonlinear neurons

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Nonlinear neurons

- ▶ Instead of step function, use differentiable function
- ▶ E.g.: use *sigmoid neurons* (*logistic neurons*)

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Nonlinear neurons

- ▶ Instead of step function, use differentiable function
- ▶ E.g.: use *sigmoid neurons* (*logistic neurons*)
- ▶ Output is sigmoid function $\sigma(z) = \frac{1}{1 + e^{-z}}$

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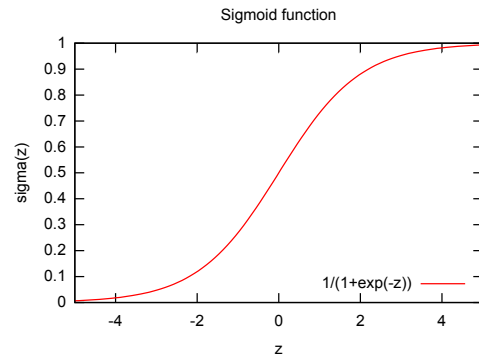
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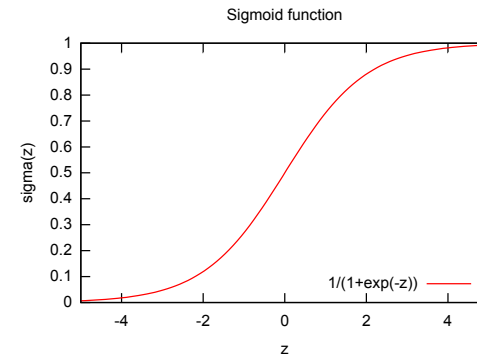
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Nonlinear neurons

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- ▶ E.g.: use *sigmoid neurons* (*logistic neurons*)
- ▶ Output is sigmoid function $\sigma(z) = \frac{1}{1 + e^{-z}}$



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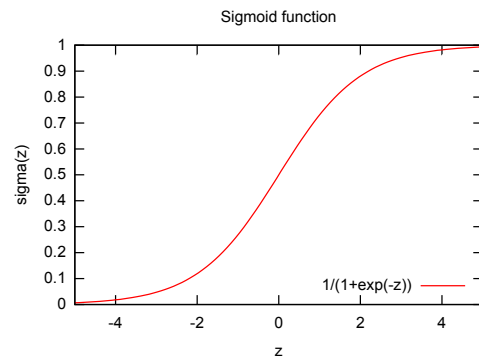
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- ▶ What is z in this case?

Nonlinear neurons

Machine Learning:
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- ▶ Instead of step function, use differentiable function
- ▶ E.g.: use *sigmoid neurons* (*logistic neurons*)
- ▶ Output is sigmoid function $\sigma(z) = \frac{1}{1 + e^{-z}}$



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- ▶ What is z in this case? \Rightarrow weighted input, bias sum

Notation changes

Machine Learning:
Part I

- ▶ Perceptron output function: only output 1 if

$$\sum_j w_j x_j + b > 0$$

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Notation changes

- ▶ Perceptron output function: only output 1 if

$$\sum_j w_j x_j + b > 0$$

- ▶ Let's represent all the w_j , x_j as **vectors** \mathbf{w} , \mathbf{x}

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Notation changes

- ▶ Perceptron output function: only output 1 if

$$\sum_j w_j x_j + b > 0$$

- ▶ Let's represent all the w_j , x_j as **vectors** \mathbf{w} , \mathbf{x}
- ▶ Now we can use **dot product** instead of summation

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Notation changes

- ▶ Perceptron output function: only output 1 if

$$\sum_j w_j x_j + b > 0$$

- ▶ Let's represent all the w_j , x_j as **vectors** \mathbf{w} , \mathbf{x}
- ▶ Now we can use **dot product** instead of summation:

$$[w_1 \ w_2 \ \cdots \ w_n] \cdot [x_1 \ x_2 \ \cdots \ x_n] = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n$$

- ▶ So perceptron outputs 1 when $\mathbf{w} \cdot \mathbf{x} + b > 0$

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Sigmoid neurons

- ▶ Sigmoid:

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

- ▶ What is z ?

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Sigmoid neurons

Machine Learning:
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- ▶ Sigmoid:

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

- ▶ What is z ?

It is the *logit*: $z = \mathbf{w} \cdot \mathbf{x} + b$

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Sigmoid neurons

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- ▶ Sigmoid:

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

- ▶ What is z ?

It is the *logit*: $z = \mathbf{w} \cdot \mathbf{x} + b$

- ▶ Small change in w or $b \Rightarrow$ small Δ in z and $\sigma(z)$

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Sigmoid neurons

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- ▶ $\sigma(z)$ is differentiable

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Sigmoid neurons

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- ▶ Small change in w or $b \Rightarrow$ small Δ in z and $\sigma(z)$

- ▶ $\sigma(z)$ is differentiable

- ▶ Δ output approximated by derivative of function at point:

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Sigmoid neurons

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► $\sigma(z)$ is differentiable

► Δ output approximated by derivative of function at point:

$$\Delta \text{output} \approx \sum_j \frac{\partial \text{output}}{\partial w_j} \Delta w_j + \frac{\partial \text{output}}{\partial b} \Delta b$$

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Sigmoid neurons

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

► What is z ?

It is the **logit**: $z = \mathbf{w} \cdot \mathbf{x} + b$

► Small change in w or $b \Rightarrow$ small Δ in z and $\sigma(z)$

► $\sigma(z)$ is differentiable

► Δ output approximated by derivative of function at point:

$$\Delta \text{output} \approx \sum_j \frac{\partial \text{output}}{\partial w_j} \Delta w_j + \frac{\partial \text{output}}{\partial b} \Delta b$$

► Now Δ output is a **linear** function of changes of weights & bias

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Incorporating the bias

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Part I

► Neuron has inputs x_i and weights w_i , $i = 1, 2, \dots, n$

► Sometimes add x_0 , w_0 to replace **bias**:

► Bias = $x_0 w_0$

► $x_0 = 1$, w_0 is learned

► $\mathbf{x} = [x_0 \ x_1 \ \dots \ x_n]^T$, $\mathbf{w} = [w_0 \ w_1 \ \dots \ w_n]^T$

► $z = \sum_{i=0}^n w_i x_i = \mathbf{w} \cdot \mathbf{x}$ is the **activation** of the neuron

► $y = f(z) = \frac{1}{1 + e^{-z}}$ is the output ("activity") of neuron

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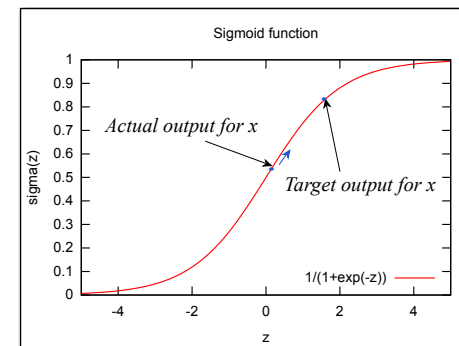
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Training a sigmoid neuron

Same basic idea as in training a perceptron:



- Want to choose Δz to move output toward target
- Determine slope at z
- Move in direction of increasing slope
- Problem: z isn't a variable: it's a dot product!
- Vector \mathbf{x} is fixed (for an example)
- So we need to change vector \mathbf{w} to move z to move toward target for same \mathbf{x}

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Derivatives of logistic neuron

- Derivative of logit z wrt. weights, inputs:

$$z = b + \sum_i w_i x_i$$
$$\frac{\partial z}{\partial w_i} = x_i, \quad \frac{\partial z}{\partial x_i} = w_i$$

- Derivative of logistic equation:

$$y = \frac{1}{1 + e^{-z}}$$
$$\frac{dy}{dz} = \frac{1}{1 + e^{-z}} \left(1 - \frac{1}{1 + e^{-z}} \right)$$
$$= y(1 - y)$$

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Derivatives of logistic neuron

- Use chain rule to differentiate y wrt w_i :

$$\frac{\partial y}{\partial w_i} = \frac{\partial z}{\partial w_i} \frac{dy}{dz} = x_i y(1 - y)$$

- Can get derivative of error wrt w_i :

$$\frac{\partial E}{\partial w_i} = \sum_n \frac{\partial y^n}{\partial w_i} \frac{\partial E}{\partial y^n} = - \sum_n x_i^n y^n (1 - y^n) (a^n - y^n)$$

where a^n means “ a from training example n ”

- First, last term \Rightarrow delta rule
- Middle term: slope of logistic equation

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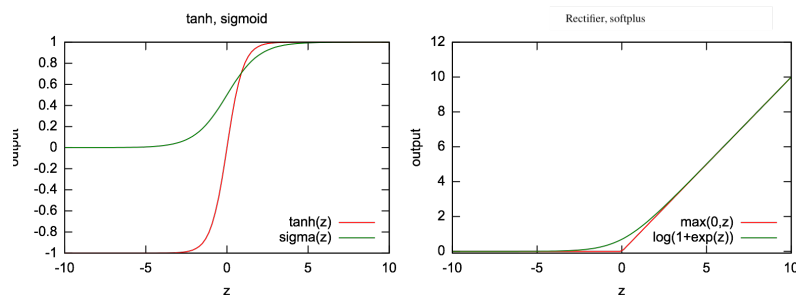
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Other non-linear neurons

- Other non-perceptron neurons possible, often used
- $\tanh(z)$, rectifier, softplus, ...



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Feedforward neural networks

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Feedforward networks

- ▶ Networks of sigmoid (or other non-perceptron) neurons
- ▶ Multiple *layers*
 - ▶ Input layer
 - ▶ Output layer
 - ▶ 1 or more *hidden layers*
- ▶ Sometimes: *multilayer perceptrons* (MLP) – though not perceptrons
- ▶ In *feedforward* net: inputs → hidden layers → outputs
- ▶ Often *dense* networks (fully-connected between layers)

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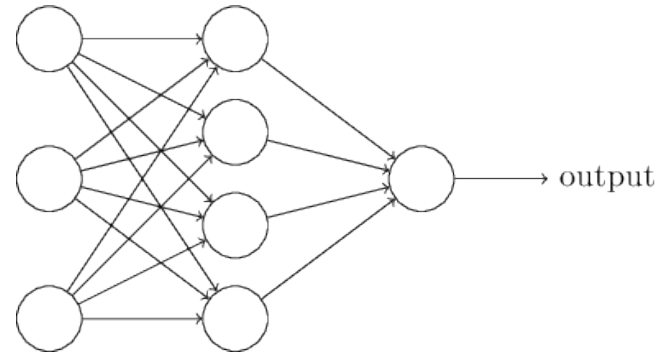


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FFN

- ▶ Could be simple, moderately complex, very complex



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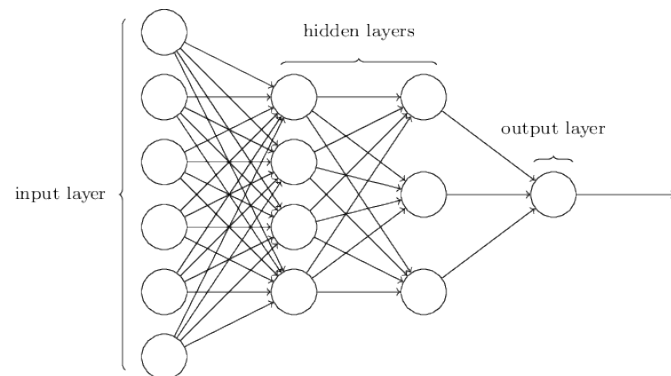


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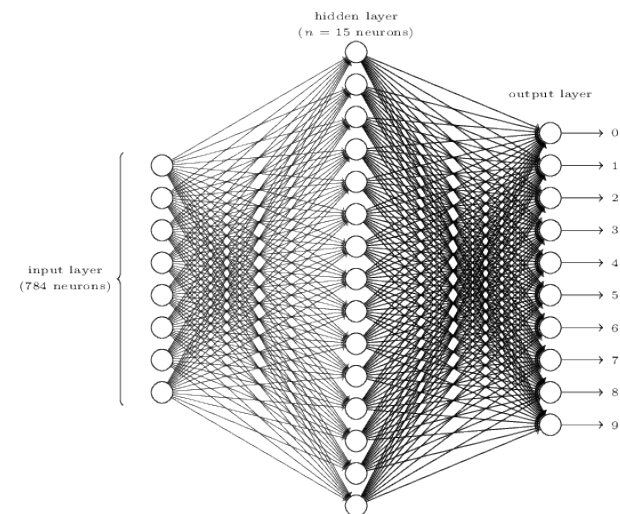


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Inputs, outputs

- ▶ Inputs?
 - ▶ “Clamped” to some activation
 - ▶ Some “natural” representation
- ▶ Outputs?
 - ▶ Classification or encoding?
 - ▶ E.g., numeral recognition:
 - ▶ Neuron for each numeral
 - ▶ Why not binary coding?

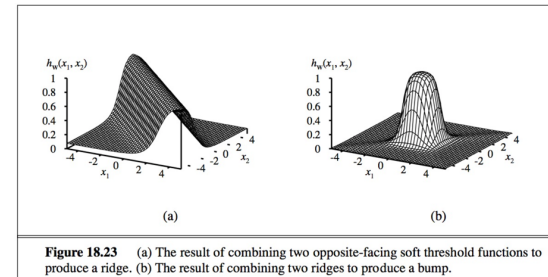
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What can FFNs learn?

- ▶ Output is composition of multiple “soft” thresholds



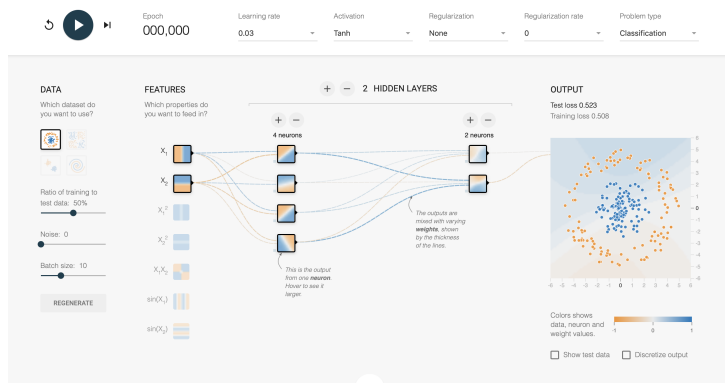
- ▶ FFN w/ single hidden layer: any continuous function, any desired precision (w/ enough neurons)
- ▶ ≥ 2 layers: discontinuous, too
- ▶ How many neurons?
 - ▶ Exponential in the inputs
 - ▶ Need $\mathcal{O}(2^n/n)$ for all Boolean functions of n inputs

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Example: NN simulator



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Matrix form of NN

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Notation (from Nielsen)

- Assume a multilayer FF network
- w_{jk}^l : wt from neuron k in layer $l - 1$ to neuron j in layer l
- Subscript: jk for ease of calculation (later)
- b_j^l : bias of neuron j in layer l

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- Assume a multilayer FF network
- w_{jk}^l : wt from neuron k in layer $l - 1$ to neuron j in layer l
- Subscript: jk for ease of calculation (later)
- b_j^l : bias of neuron j in layer l
- a_j^l : activation (output) of neuron j in layer l

$$a_j^l = \sigma \left(\sum_k w_{jk}^l a_k^{l-1} + b_j^l \right)$$

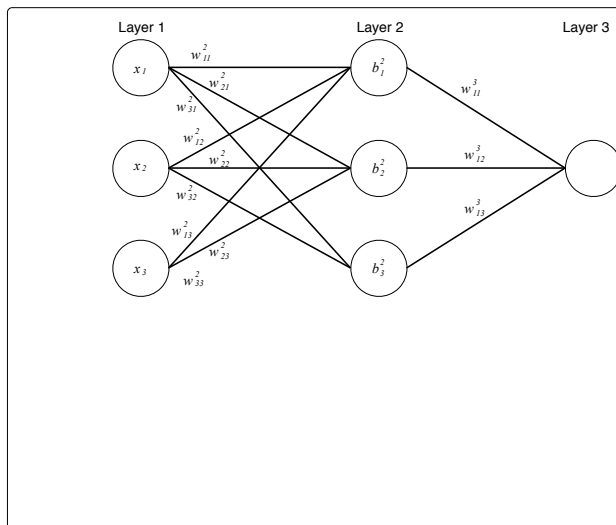
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Matrix form of NN



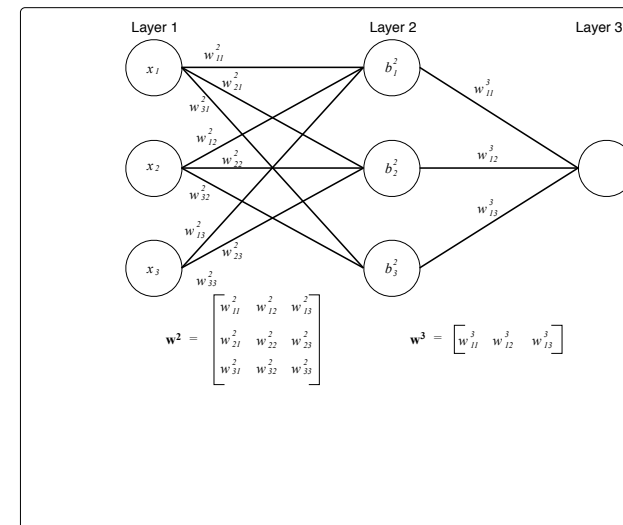
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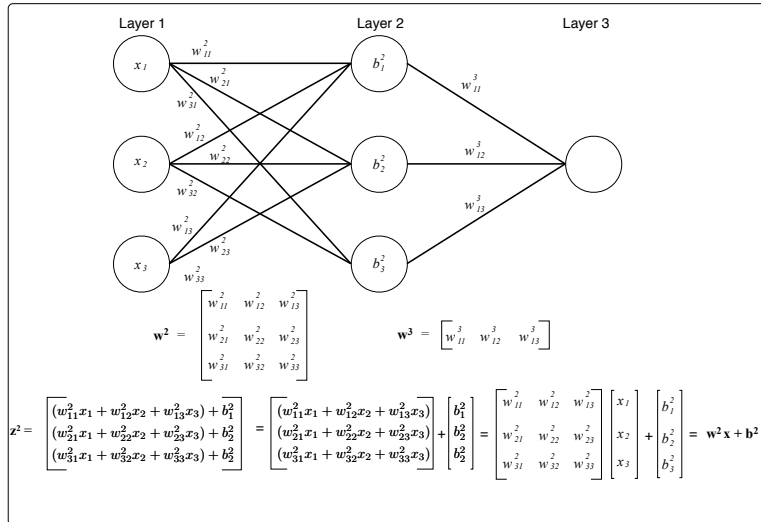
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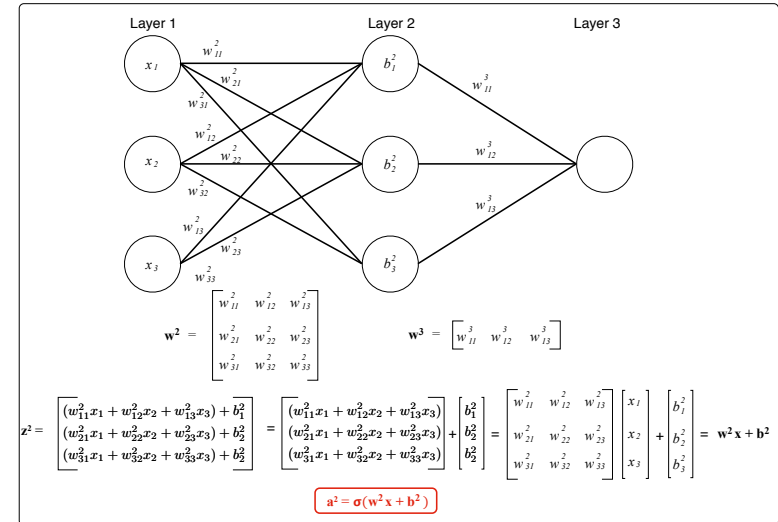
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Matrix form of NN



Matrix form of NN



Matrix form

- General equation:

$$a^l = \sigma(\mathbf{w}^l \mathbf{a}^{l-1} + \mathbf{b}^l)$$

- σ is said to be “vectorized”
- Logit (weighted input) vector \mathbf{z}^l is important, too

$$\mathbf{z}^l = \mathbf{w}^l \mathbf{a}^{l-1} + \mathbf{b}^l$$

- So $a^l = \sigma(\mathbf{z}^l)$

Gradient descent learning in FFNs

What are we learning?

Machine Learning:
Part I

- ▶ Network computes function of inputs
- ▶ Single output, n inputs \mathbf{w} : $h_{\mathbf{w}}(\mathbf{X})$
- ▶ What if $m > 1$ outputs?
 - ▶ Single layer net: separate into m nets, train separately
 - ▶ Multilayer: all outputs depend on hidden layer weights
 - ▶ \Rightarrow vector function
- ▶ Output function $\mathbf{h}_{\mathbf{w}}(\mathbf{x})$:

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$$\mathbf{h}_{\mathbf{w}}(\mathbf{x}) = \mathbf{a}^L = \sigma(\mathbf{w}^L \mathbf{a}^{L-1} + \mathbf{b}^L)$$

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Error function

Machine Learning:
Part I

- ▶ First, let's eliminate **b** \Rightarrow into **x**

- ▶ Error of network:

- ▶ Let **b** = desired output
- ▶ Error on training example **x**:

$$\mathbf{E}_w(\mathbf{x}) = \mathbf{y} - \mathbf{h}_w(\mathbf{x})$$

- ▶ But:

- ▶ $\mathbf{E}_w(\mathbf{x})$: positive/negative
- ▶ We don't want any particular error element: want *average* error
- ▶ Want to learn weights, so want a function of weights

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Cost (loss) function

Machine Learning:
Part I

- ▶ Define a *cost* (loss, objective) function:

$$C_x(\mathbf{w}) = \frac{1}{2} ||(\mathbf{E}_w(\mathbf{x}))||^2$$

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$$\begin{aligned} C_x(\mathbf{w}) &= \frac{1}{2} ||(\mathbf{E}_w(\mathbf{x}))||^2 \\ &= \frac{1}{2} ||\mathbf{y} - \mathbf{h}_w(\mathbf{x})||^2 \\ &= \frac{1}{2} \sum_m (y_m - a_m^L)^2 \end{aligned}$$

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Machine Learning:
Part I

- Define a *cost* (loss, objective) function:

$$\begin{aligned}C_{\mathbf{x}}(\mathbf{w}) &= \frac{1}{2} \|(\mathbf{E}_{\mathbf{w}}(\mathbf{x}))\|^2 \\&= \frac{1}{2} \|\mathbf{y} - \mathbf{h}_{\mathbf{w}}(\mathbf{x})\|^2 \\&= \frac{1}{2} \sum_m (y_m - a_m^L)^2\end{aligned}$$

- $C_{\mathbf{x}}(\mathbf{w})$: *quadratic cost (MSE) function*
- Entire cost function: average over all \mathbf{x}_i :

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- $C_{\mathbf{x}}(\mathbf{w})$: *quadratic cost (MSE) function*
- Entire cost function: average over all \mathbf{x}_i :

$$C(\mathbf{w}) = \frac{1}{n} \sum_i C_{\mathbf{x}_i}(\mathbf{w})$$

- Always positive, $\rightarrow 0$ as output $\rightarrow \mathbf{y}$

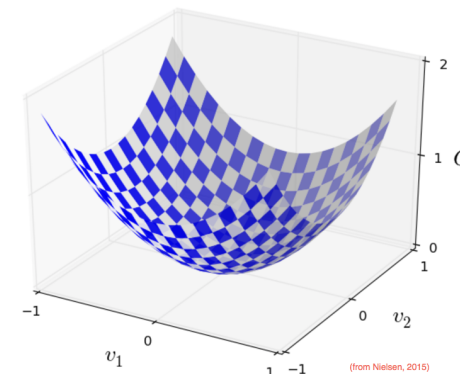
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Minimizing cost function

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- If we minimize C , minimize $\|\mathbf{E}\|$
- Using calculus, can find analytical solution
- But with n weights, $n + 1$ -dimensional curve
- E.g., two dimension:



- Largest nets: *billions* of weights

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Gradient descent search

- ▶ *Gradient descent search* instead of analytical solution
- ▶ Find *local gradients* wrt weights
- ▶ $\Rightarrow n$ *partial derivatives* of C
- ▶ Take a small step in direction of decrease in *all* the derivatives
- ▶ Repeat until close enough to minimum

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What is the local gradient?

- ▶ For simplicity: two variables, v_1, v_2

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What is the local gradient?

- ▶ For simplicity: two variables, v_1, v_2
- ▶ Then:

$$\Delta C \approx \frac{\partial C}{\partial v_1} \Delta v_1 + \frac{\partial C}{\partial v_2} \Delta v_2$$

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What is the local gradient?

- ▶ For simplicity: two variables, v_1, v_2
- ▶ Then:


$$\Delta C \approx \frac{\partial C}{\partial v_1} \Delta v_1 + \frac{\partial C}{\partial v_2} \Delta v_2$$

- ▶ Let $\Delta \mathbf{v} = [\Delta v_1 \ \Delta v_2]^T$

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- How to choose η ?
- 
- If too large \Rightarrow may overshoot minimum
- If too small \Rightarrow will take a very long time to find minimum

Computing gradient

- ▶ Difficult
- ▶ Cost function: Must compute all C_x then average

$$C = \frac{1}{n} \sum_x C_x = \frac{1}{n} \sum_x \frac{\|y(x) - a\|^2}{2}$$

- ▶ To find overall gradient ∇C :

$$\nabla C = \frac{1}{n} \sum_x \nabla C_x$$

- ▶ With many training examples, costly \Rightarrow slow learning

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Stochastic gradient descent

- ▶ Speeds up learning
- ▶ Estimate ∇C :
 - ▶ Choose small sample of inputs randomly: a *mini-batch*
 - ▶ Compute ∇C_x for these to estimate ∇C
- ▶ If batch size is large enough, average $\approx \nabla C$
- ▶ Idea:
 - ▶ Randomly partition training examples into mini-batches
 - ▶ Train with each mini-batch
- ▶ Doing this: *epoch*
- ▶ Repeat until error is satisfactory

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- ▶ Idea:
 - ▶ Randomly partition training examples into mini-batches
 - ▶ Train with each mini-batch
- ▶ Doing this: *epoch*
- ▶ Repeat until error is satisfactory
- ▶ Problem: Don't know how to calculate ∇C with hidden layers!

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Backpropagation

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Backpropagation

- ▶ *Backpropagation* algorithm (Rumelhart, Hinton, & Williams, 1986)
- ▶ Rather than trying to adjust all weights at once, do it by layers
- ▶ Compare output layer with target
- ▶ Compute error, use it to update weights from previous hidden layer to output layer
- ▶ Now propagate error in expected outputs of hidden layer backward, etc.
- ▶ Propagate by dividing responsibility for error at neuron in l according to contribution from each neuron in $l - 1$

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Error in output layer

- ▶ First define vector δ^L , where for element j :

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L)$$

where:

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Error in output layer

- ▶ First define vector δ^L , where for element j :

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L)$$

where:

- ▶ $\frac{\partial C}{\partial a_j^L}$: how fast the cost function is changing due to j 's output

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- ▶ $\sigma'(\cdot)$: 1st deriv. of $\sigma(\cdot)$

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- ▶ $\sigma'(\cdot)$: 1st deriv. of $\sigma(\cdot)$
- ▶ z_j^L : weighted input to j

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- ▶ $\sigma'(\cdot)$: 1st deriv. of $\sigma(\cdot)$
- ▶ z_j^L : weighted input to j
- ▶ Thus $\sigma'(z_j^L)$ is how fast σ is changing at z_j^L

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- ▶ $\frac{\partial C}{\partial a_j^L}$: how fast the cost function is changing due to j 's output
- ▶ $\sigma'(\cdot)$: 1st deriv. of $\sigma(\cdot)$
- ▶ z_j^L : weighted input to j
- ▶ Thus $\sigma'(z_j^L)$ is how fast σ is changing at z_j^L
- ▶ δ^L is a measure of error at L

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$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L)$$

where:

- ▶ $\frac{\partial C}{\partial a_j^L}$: how fast the cost function is changing due to j 's output
- ▶ $\sigma'(\cdot)$: 1st deriv. of $\sigma(\cdot)$
- ▶ z_j^L : weighted input to j
- ▶ Thus $\sigma'(z_j^L)$ is how fast σ is changing at z_j^L
- ▶ δ^L is a measure of error at L
- ▶ z_j^L already computed, $\sigma'(z_j^L)$ easy to compute

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Artificial
Intelligence

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Error in output layer

- First define vector δ^L , where for element j :

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L)$$

where:

- $\frac{\partial C}{\partial a_j^L}$: how fast the cost function is changing due to j 's output
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- Thus $\sigma'(z_j^L)$ is how fast σ is changing at z_j^L
- δ^L is a measure of error at L
- z_j^L already computed, $\sigma'(z_j^L)$ easy to compute
- $\frac{\partial C}{\partial a_j^L}$ for quadratic cost function: $\frac{\partial C}{\partial a_j^L} = (a_j^L - y_j)$

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Error in output layer

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where:

- $\frac{\partial C}{\partial a_j^L}$: how fast the cost function is changing due to j 's output
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- Thus $\sigma'(z_j^L)$ is how fast σ is changing at z_j^L
- δ^L is a measure of error at L
- z_j^L already computed, $\sigma'(z_j^L)$ easy to compute
- $\frac{\partial C}{\partial a_j^L}$ for quadratic cost function: $\frac{\partial C}{\partial a_j^L} = (a_j^L - y_j)$
- So for quadratic: $\delta_j^L = (a_j^L - y_j) \sigma'(z_j^L)$

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Hadamard product

- Need a new operator to simplify expressions
- Define **Hadamard product** as: $\mathbf{s} \odot \mathbf{t} = \mathbf{h}$ s.t.
 $h_j = s_j \times t_j$
- I.e., elementwise product – e.g.:

$$\begin{bmatrix} -2 \\ 20 \\ 3 \end{bmatrix} \odot \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} -6 \\ 40 \\ 3 \end{bmatrix}$$

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Error in output layer

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L)$$

- Can be rewritten as:

$$\delta^L = \nabla_a C \odot \sigma'(\mathbf{z}^L)$$

- Or

$$\delta^L = (\mathbf{a}^L - \mathbf{y}) \odot \sigma'(\mathbf{z}^L)$$

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- ▶ For each $x \in m$ training examples:
 - ▶ Feedforward: for each layer l , compute:
 - ▶ $\mathbf{z}^{x,l} = \mathbf{w}^l \mathbf{a}^{x,l-1} + \mathbf{b}^l$

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 - ▶ $\mathbf{a}^{x,l} = \sigma(\mathbf{z}^{x,l})$

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 - ▶ Compute the output error:

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 - ▶ $\delta^{x,L} = \nabla_a C_x \odot \sigma'(\mathbf{z}^{x,L})$

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 - ▶ Backpropagate error for each layer l :

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 - ▶ $\delta^{x,L} = \nabla_a C_x \odot \sigma'(\mathbf{z}^{x,L})$
 - ▶ Backpropagate error for each layer l :
 - ▶ $\delta^{x,l} = ((\mathbf{w}^{l+1})^T \delta^{x,l+1}) \odot \sigma'(\mathbf{z}^{x,l})$

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- ▶ Gradient descent: For each layer from $L \rightarrow 2$:

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 - ▶ $\delta^{x,L} = \nabla_a C_x \odot \sigma'(\mathbf{z}^{x,L})$
 - ▶ Backpropagate error for each layer l :
 - ▶ $\delta^{x,l} = ((\mathbf{w}^{l+1})^T \delta^{x,l+1}) \odot \sigma'(\mathbf{z}^{x,l})$
- ▶ Gradient descent: For each layer from $L \rightarrow 2$:
 - ▶ Next $\mathbf{w}^l = \mathbf{w}^l - \frac{\eta}{m} \sum_x \delta^{x,l} (\mathbf{a}^{x,l-1})^T$

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Do for some # of epochs, some # mini-batches each.

Backprop algorithm

Machine Learning:
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```

function BACK-PROP-LEARNING(examples, network) returns a neural network
  inputs: examples, a set of examples, each with input vector  $\mathbf{x}$  and output vector  $\mathbf{y}$ 
           network, a multilayer network with  $L$  layers, weights  $w_{i,j}$ , activation function  $g$ 
  local variables:  $\Delta$ , a vector of errors, indexed by network node

  repeat
    for each weight  $w_{i,j}$  in network do
       $w_{i,j} \leftarrow$  a small random number
    for each example  $(\mathbf{x}, \mathbf{y})$  in examples do
      /* Propagate the inputs forward to compute the outputs */
      for each node  $i$  in the input layer do
         $a_i \leftarrow x_i$ 
      for  $\ell = 2$  to  $L$  do
        for each node  $j$  in layer  $\ell$  do
           $in_j \leftarrow \sum_i w_{i,j} a_i$ 
           $a_j \leftarrow g(in_j)$ 
      /* Propagate deltas backward from output layer to input layer */
      for each node  $j$  in the output layer do
         $\Delta[j] \leftarrow g'(in_j) \times (y_j - a_j)$ 
      for  $\ell = L - 1$  to  $1$  do
        for each node  $i$  in layer  $\ell$  do
           $\Delta[i] \leftarrow g'(in_i) \sum_j w_{i,j} \Delta[j]$ 
      /* Update every weight in network using deltas */
      for each weight  $w_{i,j}$  in network do
         $w_{i,j} \leftarrow w_{i,j} + \alpha \times a_i \times \Delta[j]$ 
  until some stopping criterion is satisfied
  return network
    
```

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- ▶ Networks with ≥ 2 hidden layers are *deep networks*
- ▶ Backprop will still work for them
- ▶ But:

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 - ▶ Tend to lose the error “signal” as propagate back through network

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 - ▶ Each neuron in earlier layers have less and less impact on output error

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 - ▶ *Vanishing gradient problem*

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 - ▶ *Vanishing gradient problem*
- ▶ \Rightarrow *extremely* slow learning rate

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- ▶ \Rightarrow *extremely* slow learning rate
- ▶ Can have opposite problem, depending on net: *exploding gradient problem*

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- ▶ Stymied researchers for many years – until

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 - ▶ Faster machines
 - ▶ Better versions of backprop-ish algorithms invented

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 - ▶ Better versions of backprop-ish algorithms invented
- ▶ \Rightarrow tremendous increase in deep learning research, applications

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- ▶ Stymied researchers for many years – until
 - ▶ Faster machines
 - ▶ Better versions of backprop-ish algorithms invented
- ▶ \Rightarrow tremendous increase in deep learning research, applications
- ▶ We'll come back to this later in course

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Neural network training:
... and ...
What can they do?
How do they work?
Autoencoders
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Deep learning nets
Building them: Keras, TensorFlow, PyTorch, etc.

Neural network training:

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"You process a lot of data in a quiet way, don't you, Larry!"



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... and ...

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You'd like to ask Roy if he's really thought this through.



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- Neural network training:
 - ... and ...
 - What can they do?
 - How do they work?
 - Autoencoders
 - Restricted Boltzmann machines**
 - Feed-forward NN
 - Deep learning nets
 - Building them: Keras, TensorFlow, PyTorch, etc.



Machine Learning:
Part I

Summary

Feed-forward NN

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Deep learning nets

Artificial Intelligence

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Deep learning

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