Introduction to Artificial Neural Networks

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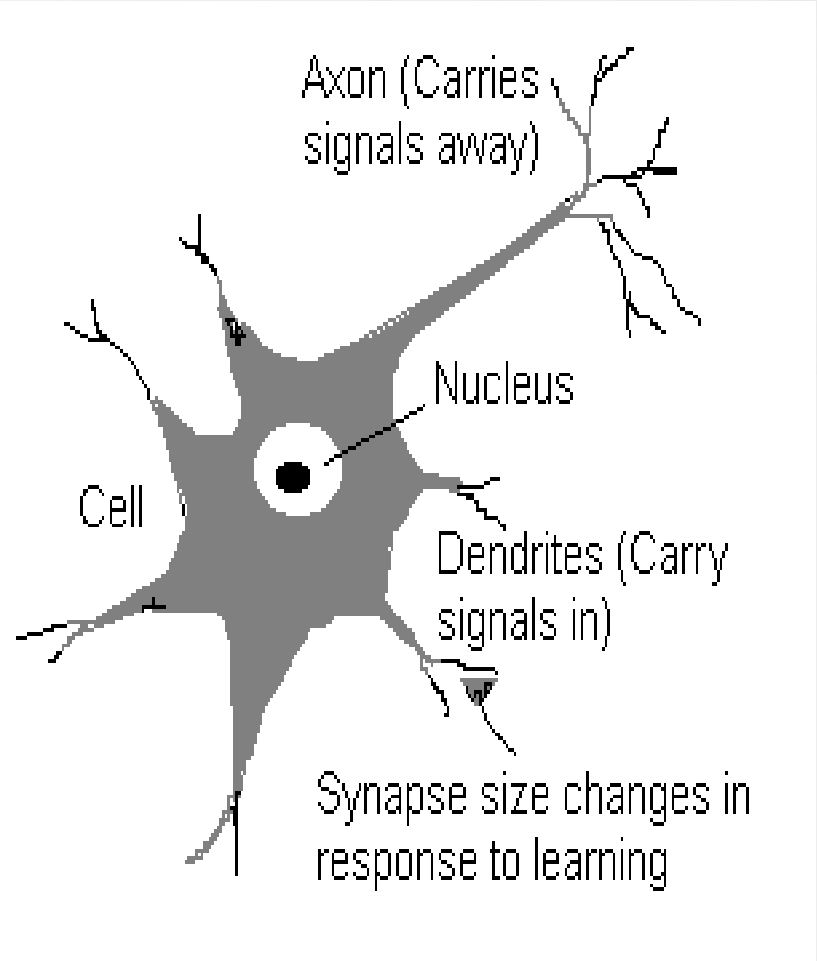
Lecture Outline

- **The Perceptron**
- **Multi-Layer Networks**
  - Nonlinear transfer functions
  - Multi-layer networks of nonlinear units (sigmoid, hyperbolic tangent)
- **Backpropagation of Error**
  - The backpropagation algorithm
  - Training issues
    - Convergence
    - Overfitting
- **Hidden-Layer Representations**
- **Examples: Face Recognition and Text-to-Speech**
- **Backpropagation and Faster Training**
- **Some Open problems**

In the beginning was … the Neuron!

- A neuron (nervous system cell): many-inputs / one-output unit
- output can be *excited* or *not excited*
- incoming signals from other neurons determine if the neuron shall excite ("fire")
- The output depends on the attenuations occuring in the *synapses:* parts where a neuron communicates with another



The Synapse Concept

- The synapse resistance to the incoming signal can be changed during a "learning" process [Hebb, 1949]

Hebb's Rule:

If an input of a neuron is repeatedly and persistently causing the neuron to fire, then a metabolic change happens in the synapse of that particular input to reduce its resistance

Connectionist (Neural Network) Models

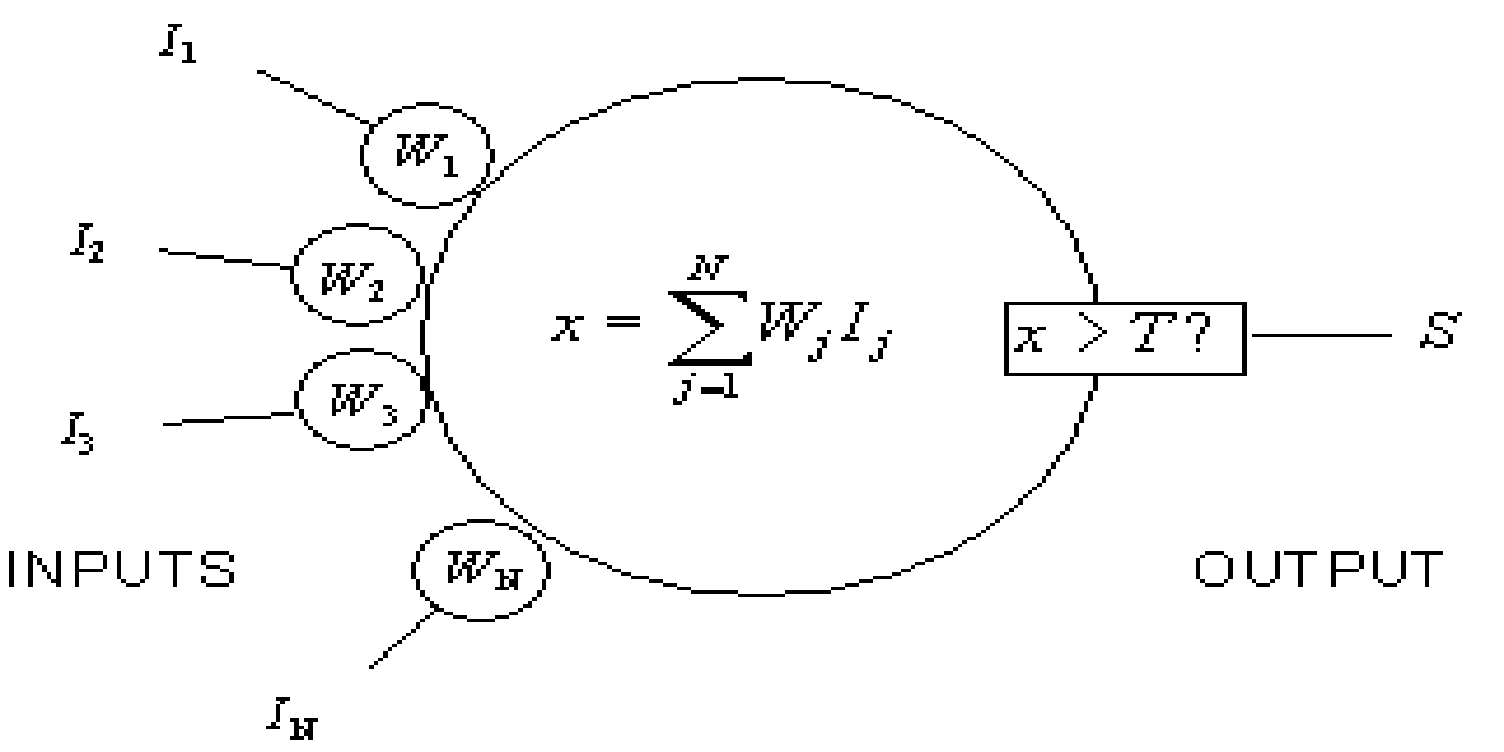
- **Human Brain**
  - Number of neurons: ~100 billion (10^{11})
  - Connections per neuron: ~10-100 thousand (10^4 – 10^5)
  - Neuron switching time: ~ 0.001 (10^{-3}) second
  - Scene recognition time: ~0.1 second
  - 100 inference steps doesn't seem sufficient!

    ➔ Massively parallel computation

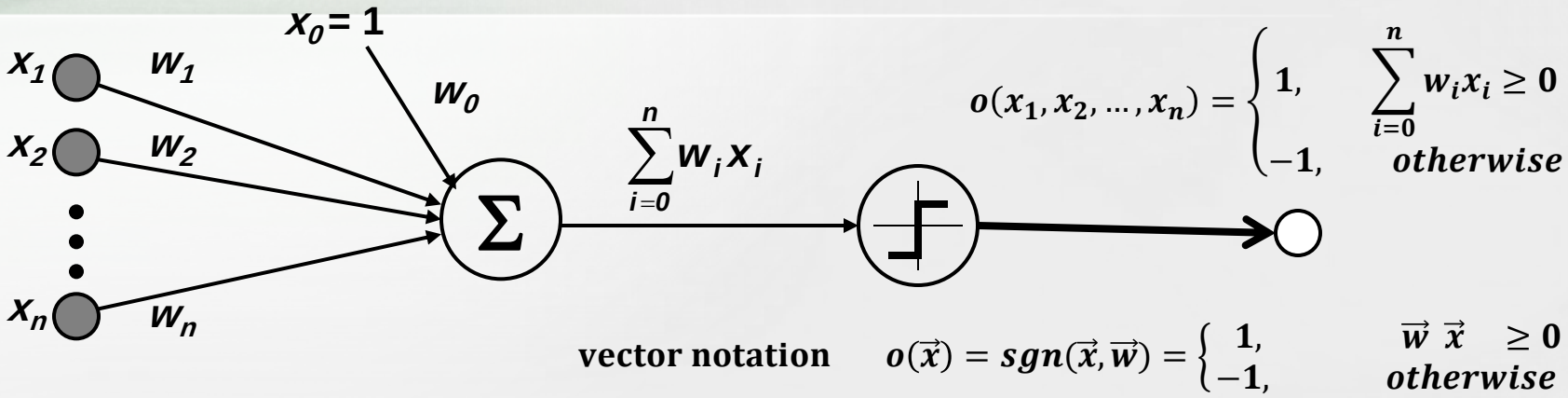
- (List of animals by number of neurons: https://en.wikipedia.org/wiki/List_of_animals_by_number_of_neurons)

Mathematical Modelling

The neuron calculates a weighted **x** (or **net**) sum of inputs and compares it to a threshold **T**. If the sum is higher than the threshold, the output **S** is set to 1, otherwise to -1.



The Perceptron

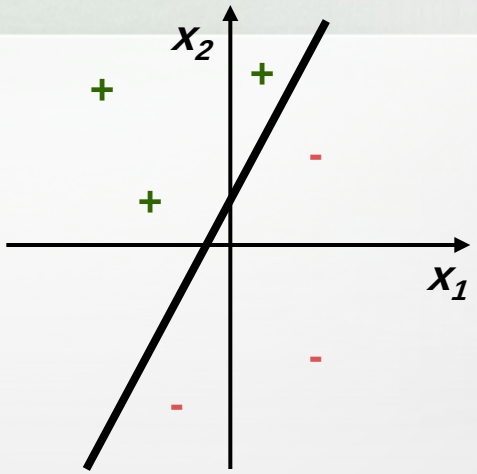


- **Perceptron: Single Neuron Model**
  - Linear Threshold Unit (LTU) or Linear Threshold Gate (LTG)
  - Net input to unit: defined as a linear combination $net(x) = \sum_{i=0}^{n} w_i x_i$
  - Output of unit: threshold (activation) function on net input (threshold $\theta = -w_0$)
- **Perceptron Networks**
  - Neuron is modeled using a unit connected by weighted links w_i to other units
  - Multi-Layer Perceptron (MLP)

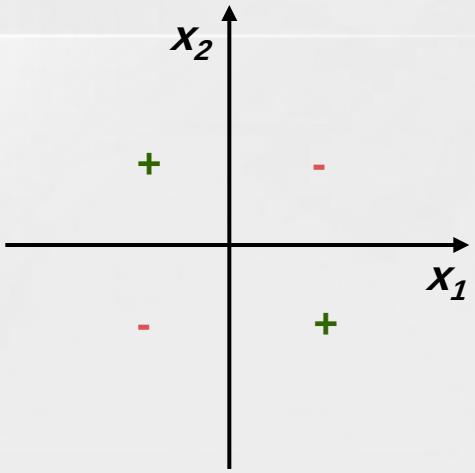
Connectionist (Neural Network) Models

- **Definitions of Artificial Neural Networks (ANNs)**
  - "… a system composed of many simple processing elements operating in parallel whose function is determined by network structure, connection strengths, and the processing performed at computing elements or nodes." - DARPA (1988)
- **Properties of ANNs**
  - Many neuron-like threshold switching units
  - Many weighted interconnections among units
  - Highly parallel, distributed process
  - Emphasis on tuning weights automatically

Decision Surface of a Perceptron



Example A



Example B

- **Perceptron: Can Represent *Some* Useful Functions (And, Or, Nand, Nor)**
  - LTU emulation of logic gates (McCulloch and Pitts, 1943)
  - e.g., What weights represent $g(x_1, x_2) = AND(x_1, x_2)$? $OR(x_1, x_2)$? $NOT(x)$?

    ($w_0 + w_1 \cdot x_1 + w_2 \cdot x_2$ $w_0 = -0.8$ $w_1 = w_2 = 0.5$ $w_0 = -0.3$)
- **Some Functions are *Not* Representable**
  - e.g., not linearly separable
  - Solution: use networks of perceptrons (LTUs)

Learning Rules for Perceptrons

- **Learning Rule ≡ Training Rule**
  - Not specific to supervised learning
  - Idea: Gradual building/update of a model
- **Hebbian Learning Rule (Hebb, 1949)**
  - Idea: if two units are both active ("firing"), weights between them should increase
  - $w_{ij} = w_{ij} + r\, o_i\, o_j$

    where r is a learning rate constant
  - Supported by neuropsychological evidence

Learning Rules for Perceptrons

- **Perceptron Learning Rule (Rosenblatt, 1959)**
  - **Idea**: when a target output value is provided for a single neuron with fixed input, it can incrementally update weights to learn to produce the output
  - Assume binary (boolean-valued) input/output units; single LTU
  - $$w_i \leftarrow w_i + \Delta w_i$$

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

    where $t = c(x)$ is target output value, o is perceptron output, r is small learning rate constant (e.g., 0.1)
  - Convergence proven for D linearly separable and r small enough

Perceptron Learning Algorithm

- **Simple Gradient Descent Algorithm**
  - Applicable to concept learning, symbolic learning (with proper representation)
- **Algorithm *Train-Perceptron* ($D \equiv \{<x, t(x) \equiv c(x)>\}$)**
  - Initialize all weights w_i to random values
  - WHILE not all examples correctly predicted DO

    FOR each training example $x \in D$

    Compute current output $o(x)$

    FOR $i = 1$ to n

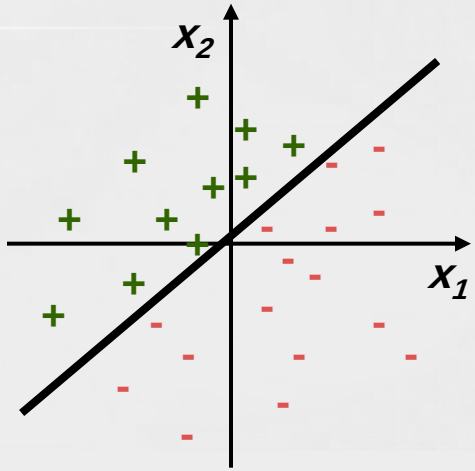
    $w_i \leftarrow w_i + r(t - o)x_i$ // perceptron learning rule

Perceptron Learning Algorithm

- **Perceptron Learnability**
  - Recall: can only learn $h \in H$ - i.e., linearly separable (LS) functions
  - Minsky and Papert, 1969: demonstrated representational limitations
    - e.g., parity (n-attribute XOR: $x_1 \oplus x_2 \oplus \ldots \oplus x_n$)
    - e.g., symmetry, connectedness in visual pattern recognition
    - Influential book *Perceptrons* discouraged ANN research for ~10 years
  - NB: "Can we transform learning problems into LS ones?"

Linear Separators

- **Functional Definition**
  - $f(x) = 1$ if $w_1x_1 + w_2x_2 + \ldots + w_nx_n \geq \theta$, 0 otherwise
  - θ: threshold value



Linearly Separable (LS) Data Set

- **Non Linearly Separable Functions**
  - Disjunctions: $c(x) = x_1' \vee x_2' \vee \ldots \vee x_m'$
  - m of n: $c(x)$ = at least 3 of $(x_1', x_2', \ldots, x_m')$
  - Exclusive OR (XOR): $c(x) = x_1 \oplus x_2$
  - General DNF: $c(x) = T_1 \vee T_2 \vee \ldots \vee T_m$; $T_i = l_1 \wedge l_2 \wedge \ldots \wedge l_k$
- **Change of Representation Problem**
  - Can we transform non-LS problems into LS ones?
  - Is this meaningful? Practical?
  - Does it represent a significant fraction of real-world problems?

Perceptron Convergence

- **Perceptron Convergence Theorem**
  - Claim: If there exists a set of weights that are consistent with the data (i.e., the data is linearly separable), the perceptron learning algorithm will converge
  - Caveat 1: How long will this take?
  - Caveat 2: What happens if the data is *not* LS?
- **Perceptron Cycling Theorem**
  - Claim: If the training data is not LS the perceptron learning algorithm will eventually repeat the same set of weights and thereby enter an infinite loop
- **How to Provide More Robustness, Expressivity?**
  - Objective 1: develop algorithm that will find closest approximation
  - Objective 2: develop architecture to overcome representational limitation

Gradient Descent: Principle

- **Understanding Gradient Descent for Linear Units**
  - Consider simpler, unthresholded linear unit:

$$o(\vec{x}) = net(x) = \sum_{i=0}^{n} w_i x_i$$

  - Objective: find "best fit" to *D*
- **Approximation Algorithm**
  - Quantitative objective: minimize error over training data set *D*
  - Error function: sum squared error (SSE)

$$E(\vec{w}) = Error_D(\vec{w}) = \frac{1}{2} \sum_{x \in D} (t(x) - o(x))^2$$

- **How to Minimize?**
  - Simple optimization
  - Move in direction of steepest gradient in weight-error space
    - Computed by finding tangent
    - i.e. partial derivatives (of *E*) with respect to weights (w_i)

Gradient Descent: Derivation of Delta/LMS (Widrow-Hoff) Rule

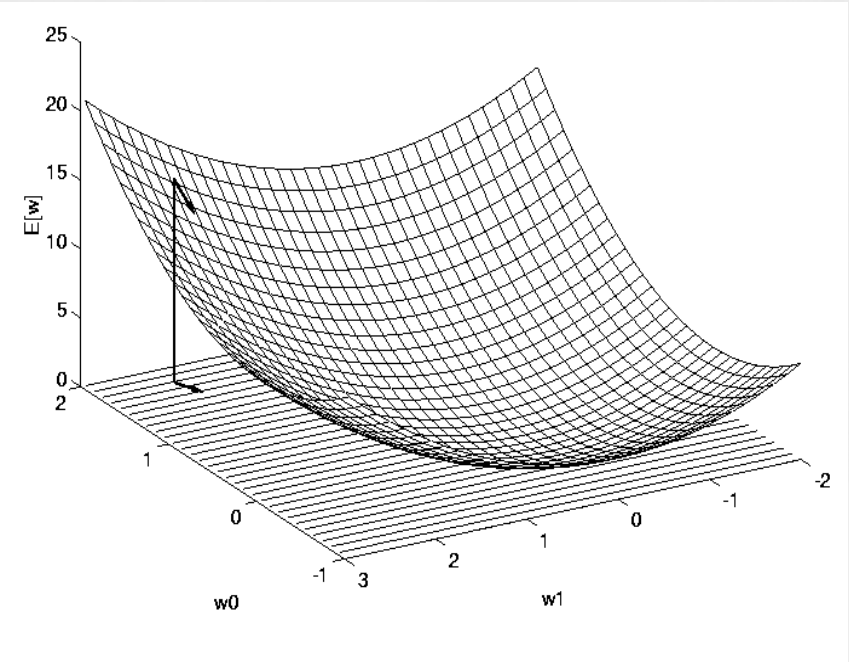
- **Definition: Gradient**

$$\nabla E(\vec{w}) = \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \ldots, \frac{\partial E}{\partial w_n}\right]$$

- **Modified Gradient Descent Training Rule**

$$\Delta \vec{W} = -r\, \nabla E(\vec{w})$$

$$\Delta w_i = -r\, \frac{\partial E}{\partial w_i}$$



$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i}\left[\frac{1}{2}\sum_{x \in D}\big(t(x) - o(x)\big)^2\right] = \left[\frac{1}{2}\sum_{x \in D}\frac{\partial}{\partial w_i}\big(t(x) - o(x)\big)^2\right]$$

$$\frac{\partial E}{\partial w_i} = \frac{1}{2}\sum_{x \in D}\left[2\big(t(x) - o(x)\big)\frac{\partial}{\partial w_i}\big(t(x) - o(x)\big)\right] = \sum_{x \in D}\left[\big(t(x) - o(x)\big)\frac{\partial}{\partial w_i}(t(x) - \vec{w}\ \vec{x})\right]$$

$$\frac{\partial E}{\partial w_i} = \sum_{x \in D}\left[\big(t(x) - o(x)\big)(-x_i)\right]$$

Gradient Descent: Algorithm using Delta/LMS Rule

- **Algorithm *Gradient-Descent* (*D*, *r*)**
  - Each training example is a pair of the form $<x, t(x)>$, where x: input vector; $t(x)$: target vector; r :learning rate
  - Initialize all weights w_i to (small) random values
  - UNTIL the termination condition is met, DO

    Initialize each Δw_i to zero

    FOR each instance $<x, t(x)>$ in D, DO

    Input x into the unit and compute output o

    FOR each linear unit weight w_i, DO

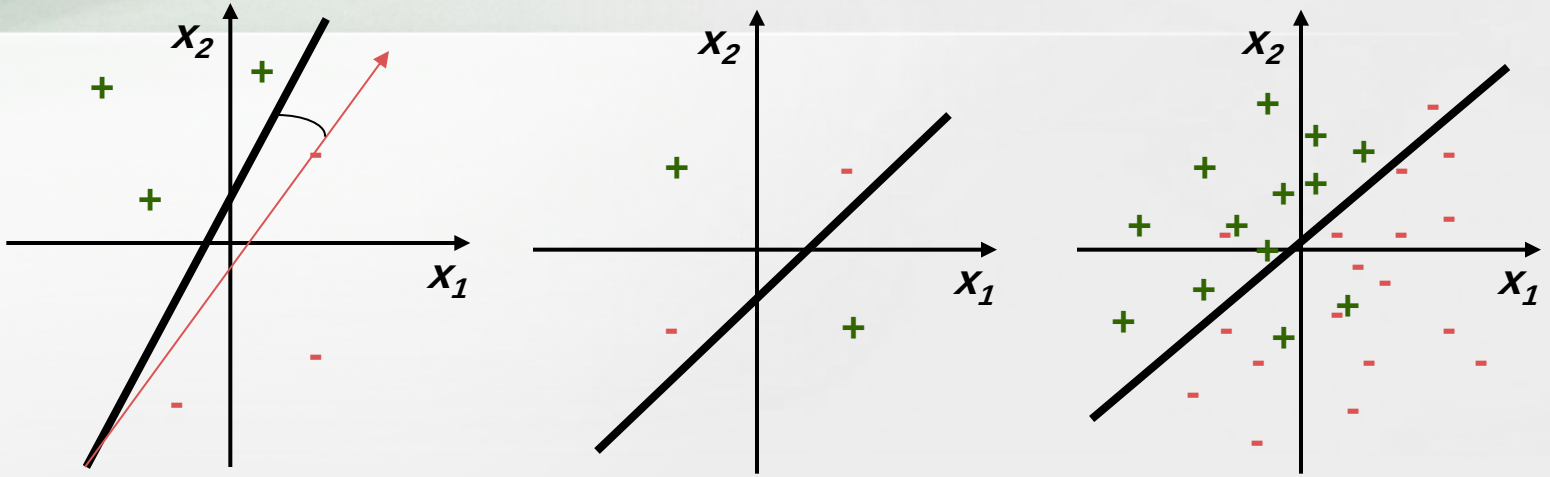
    $\Delta w_i \leftarrow \Delta w_i + r(t - o)x_i$

    $w_i \leftarrow w_i + \Delta w_i$
  - RETURN final w

Gradient Descent: Algorithm using Delta/LMS Rule

- **Mechanics of Delta Rule**
  - Gradient is based on a derivative
  - Significance: later, we will use nonlinear activation functions (*aka* transfer functions, squashing functions)

Gradient Descent: Perceptron Rule versus Delta/LMS Rule



Example A Example B Example C

- **LS Concepts: Can Achieve Perfect Classification**
  - Example A: perceptron training rule converges
- **Non-LS Concepts: Can Only Approximate**
  - Example B: not LS; delta rule converges, but can't do better than 3 correct
  - Example C: not LS; better results from delta rule

Incremental (Stochastic) Gradient Descent

- **Batch Mode Gradient Descent**
  - UNTIL the termination condition is met, DO
    1. Compute the gradient $\nabla E_D(\vec{w})$
    2. Update the weights $\vec{w} \leftarrow \vec{w} - r\,\nabla E_D(\vec{w})$
  - RETURN final *w*
- **Incremental (Online) Mode Gradient Descent**
  - UNTIL the termination condition is met, DO

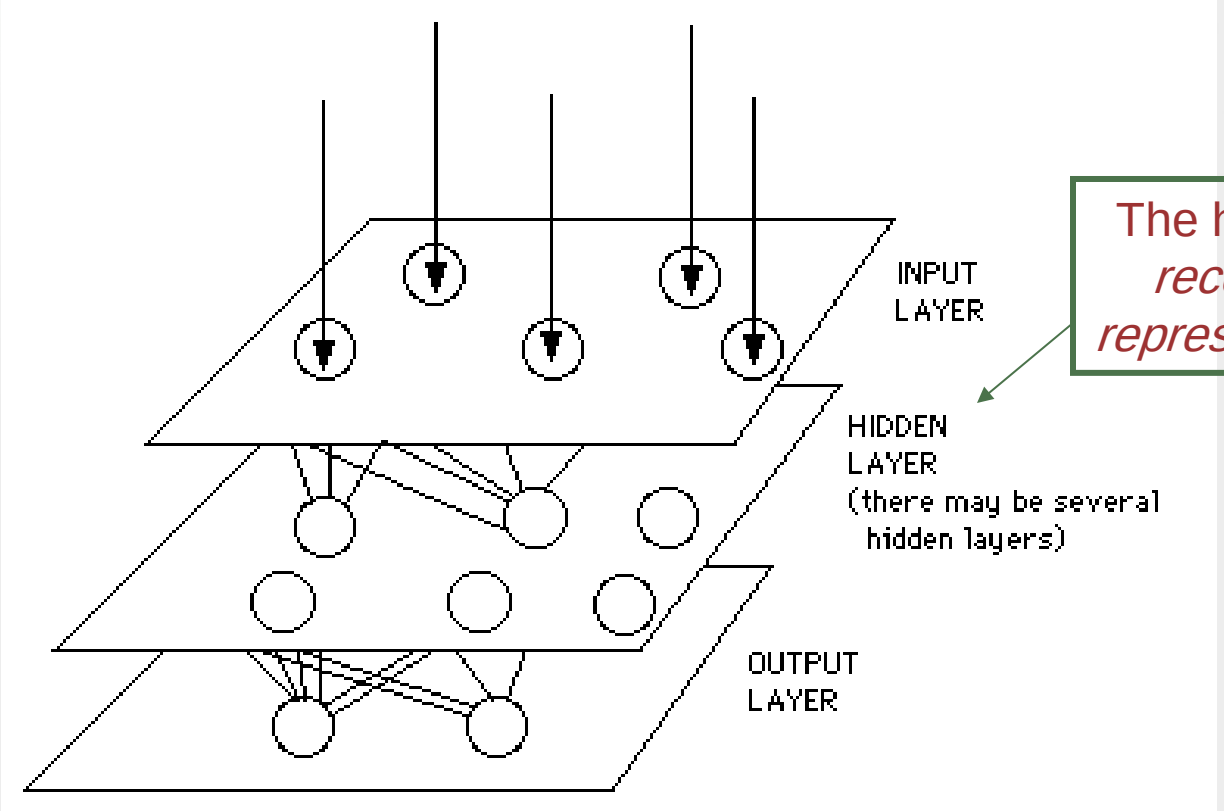
    FOR each <*x*, *t*(*x*)> in *D*, DO
    1. Compute the gradient $\nabla E_d(\vec{w})$
    2. Update the weights $\vec{w} \leftarrow \vec{w} - r\,\nabla E_d(\vec{w})$
  - RETURN final *w*
- **Emulating Batch Mode**
  - $$E_D[\vec{w}] \equiv \frac{1}{2}\left[\sum_{x \in D}(t(x) - o(x))^2\right], \quad E_d[\vec{w}] \equiv \frac{1}{2}(t(x) - o(x))^2$$
  - Incremental gradient descent can approximate batch gradient descent arbitrarily closely if *r* made small enough

GD vs Stochastic GD

- **Gradient Descent**
  - Converges to a weight vector with minimal error regardless whether D is Lin. Separable, given a sufficiently small learning rate is used.
  - Difficulties:
    - Convergence to local minimum can be slow
    - No guarantee to find global minimum
- **Stochastic Gradient Descent** intended to alleviate these difficulties
- Differences
  - In Standard GD, error summed over D before updating W
  - In Standard GD, more computation per weight update step (but larger step size per weight update)
  - Stochastic GD can sometimes avoid falling into local minima
- Both commonly used in Practice

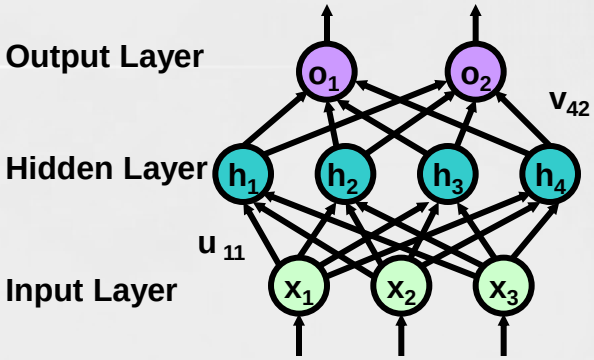
Artificial Neural Networks

Adaptive interaction between individual neurons
Power: collective behavior of interconnected neurons



The hidden layer learns to *recode* (or to *provide a representation* of) the inputs

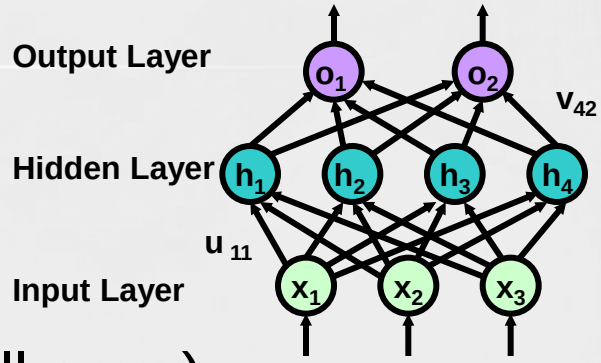
Multi-Layer Networks of Nonlinear Units



- **Nonlinear Units**
  - Recall: activation function *sgn* ($w \bullet x$)
  - Nonlinear activation function: generalization of *sgn*

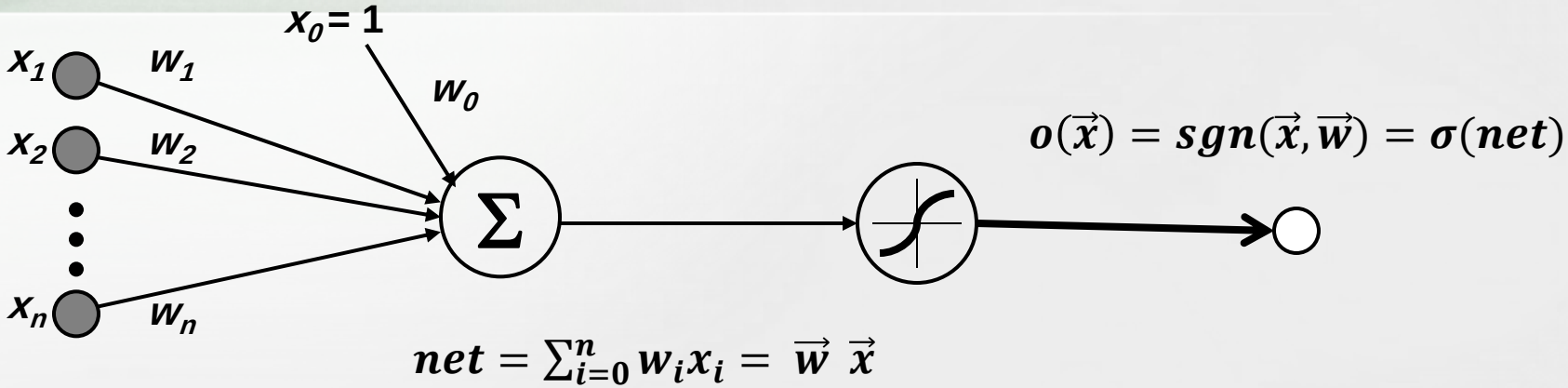
- **Multi-Layer Networks**
  - A specific type: Multi-Layer Perceptrons (MLPs)
  - Definition: a multi-layer feedforward network is composed of an input layer, one or more hidden layers, and an output layer
  - Only hidden and output layers contain perceptrons (threshold or nonlinear units)

Multi-Layer Networks of Nonlinear Units

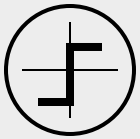


- **MLPs in Theory**
  - Network (of 2 or more layers) can represent any function (arbitrarily small error)
  - Training even 3-unit multi-layer ANNs is NP-hard (Blum and Rivest, 1992)
- **MLPs in Practice**
  - Finding or *designing* effective networks for arbitrary functions is difficult
  - Training is very computation-intensive even when structure is "known"

Nonlinear Activation Functions



- **Sigmoid Activation Function**



  - Linear threshold gate activation function: *sgn* (*w* • *x*)
  - Nonlinear activation (*aka* transfer, squashing) function: generalization of *sgn*
  - σ is the sigmoid function $\sigma(net) = \frac{1}{1+e^{-net}}$
  - Can derive gradient rules to train
    - One sigmoid unit
    - Multi-layer, feedforward networks of sigmoid units (using backpropagation)
- **Hyperbolic Tangent Activation Function** $\sigma(net) = \frac{\sinh(net)}{\cosh(net)} = \frac{e^{net} - e^{-net}}{e^{net} + e^{-net}}$

Error Gradient for a Sigmoid Unit

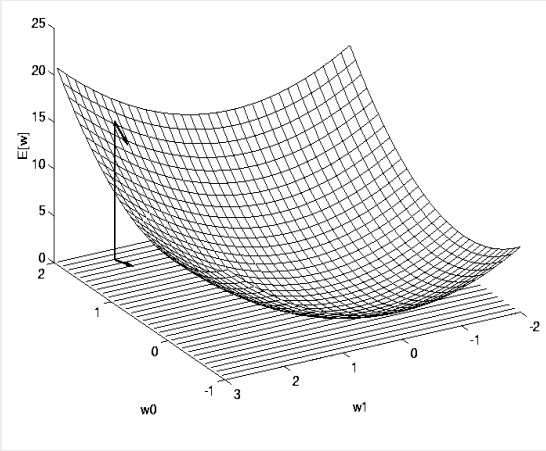
- **Recall: Gradient of Error Function** $\nabla E(\vec{w}) = \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \ldots, \frac{\partial E}{\partial w_n}\right]$
- **Gradient of Sigmoid Activation Function**

$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i}\left[\frac{1}{2}\sum_{\langle \vec{x}|t(\vec{x})\rangle \in D}\left(t(\vec{x}) - o(\vec{x})\right)^2\right] = \left[\frac{1}{2}\sum_{\langle \vec{x}|t(\vec{x})\rangle \in D}\frac{\partial}{\partial w_i}\left(t(\vec{x}) - o(\vec{x})\right)^2\right] =$$

$$= \frac{1}{2}\sum_{\langle \vec{x}|t(\vec{x})\rangle \in D}\left[2\left(t(\vec{x}) - o(\vec{x})\right)\frac{\partial}{\partial w_i}\left(t(\vec{x}) - o(\vec{x})\right)\right]$$

$$= \sum_{\langle \vec{x}|t(\vec{x})\rangle \in D}\left[\left(t(\vec{x}) - o(\vec{x})\right)\left(-\frac{\partial}{\partial w_i}o(\vec{x})\right)\right]$$

$$= -\sum_{\langle \vec{x}|t(\vec{x})\rangle \in D}\left[\left(t(\vec{x}) - o(\vec{x})\right)\left(\frac{\partial o(\vec{x})}{\partial net(\vec{x})}\frac{\partial net(\vec{x})}{\partial w_i}\right)\right]$$



- **But we know:**

$$\frac{\partial o(\vec{x})}{\partial net(\vec{x})} = \frac{\partial \sigma(\overrightarrow{net})}{\partial net(\vec{x})} = \left(o(\vec{x})\right)\left(1 - o(\vec{x})\right) \qquad \frac{\partial net(\vec{x})}{\partial w_i} = \frac{\partial(\vec{w}\ \vec{x})}{\partial w_i} = x_i$$

So:

$$\frac{\partial E}{\partial w_i} = \sum_{\langle \vec{x}|t(\vec{x})\rangle \in D}\left[\left(t(\vec{x}) - o(\vec{x})\right)\left(o(\vec{x})\right)\left(1 - o(\vec{x})\right)x_i\right]$$

The Backpropagation Algorithm

- **Intuitive Idea: Distribute the *Blame* for Error to the Previous Layers**
- **Algorithm *Train-by-Backprop* (*D*, *r*)**
  - Each training example is a pair of the form $\langle x, t(x) \rangle$, where x: input vector; $t(x)$: target vector; r :learning rate
  - Initialize all weights w_i to (small) random values
  - UNTIL the termination condition is met, DO

    FOR each $\langle x, t(x) \rangle$ in D, DO

      Input the instance x to the unit and compute the output $o(x) = \sigma(net(x))$

      FOR each output unit k, DO (calculate its error)

$$\delta_k = o_k(x)(1 - o_k(x))(t_k(x) - o_k(x))$$

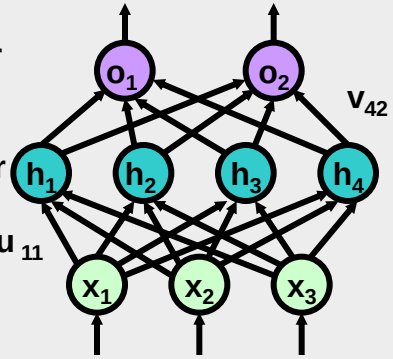
      FOR each hidden unit j, DO

$$\delta_j = h_j(x)(1 - h_j(x)) \sum_{k \in outputs} v_{j,k}\delta_k$$

      Update each $w = u_{i,j}$ $(a = h_j)$ or $w = v_{j,k}$ $(a = o_k)$

$$w_{start\text{-}layer,\ end\text{-}layer} \leftarrow w_{start\text{-}layer,\ end\text{-}layer} + \Delta w_{start\text{-}layer,\ end\text{-}layer}$$

$$\Delta w_{start\text{-}layer,\ end\text{-}layer} \leftarrow r\,\delta_{end\text{-}layer}\,a_{end\text{-}layer}$$



  - RETURN final u, v

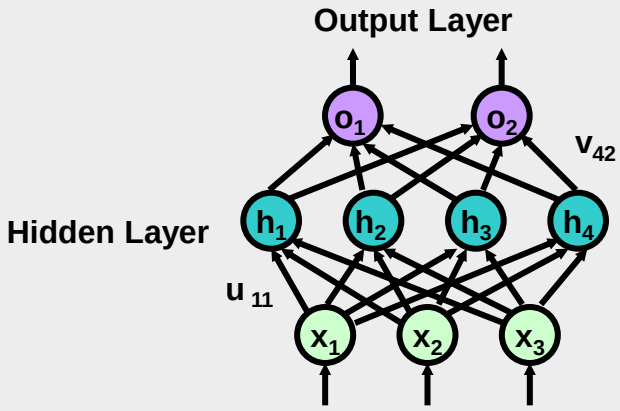
The Backpropagation Algorithm (1)

- **Algorithm *Train-by-Backprop* (*D*, *r*)**
  - *D* is a set of training examples of the form <*x*, *t*(*x*)>, where

    x: input vector;

    t(x): target vector;

    r :learning rate
  - Initialize all weights w_i to (small) random values
  - UNTIL the termination condition is met, DO



The Backpropagation Algorithm (cont.)

FOR each <x, $t(x)$> in D, DO

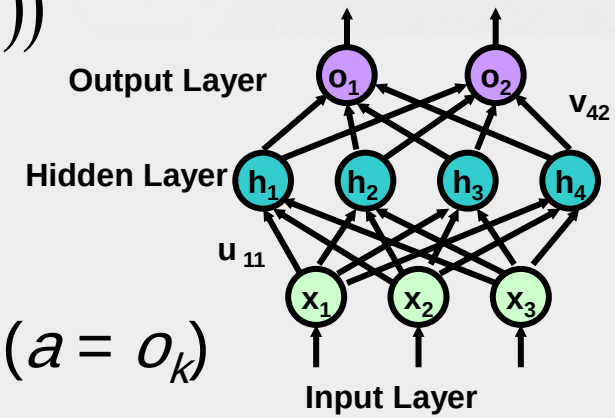
Input the instance x to the unit and compute the output $o(x)$ $= \sigma(net(x))$

FOR each output unit k, DO (calculate its error)

$$\delta_k = o_k(x)(1-o_k(x))(t_k(x)-o_k(x))$$

FOR each hidden unit j, DO

$$\delta_j = h_j(x)(1-h_j(x)) \sum_{k \in outputs} v_{j,k}\delta_k$$



Update each $w = u_{i,j}$ $(a = h_j)$ or $w = v_{j,k}$ $(a = o_k)$

$$w_{start\text{-}layer,\ end\text{-}layer} \leftarrow w_{start\text{-}layer,\ end\text{-}layer} + \Delta w_{start\text{-}layer,\ end\text{-}layer}$$

$$\Delta w_{start\text{-}layer,\ end\text{-}layer} \leftarrow r\,\delta_{end\text{-}layer}\,a_{end\text{-}layer}$$

– RETURN final u, v

Backpropagation and Local Optima

- **Gradient Descent in Backprop**
  - Performed over entire *network* weight vector
  - Easily generalized to arbitrary directed graphs
  - Property: Backpropagation on feedforward ANNs will find a *local* (not necessarily global) error minimum

Backpropagation and Local Optima

- **Backprop in Practice**
  - Local optimization often works well (can *run multiple times*)
  - A weight momentum α is often included:

$$\Delta w_{start\text{-}layer,end\text{-}layer}(n) = r\,\delta_{end\text{-}layer}\,a_{end\text{-}layer} + \alpha\Delta w_{start\text{-}layer,end\text{-}layer}(n-1)$$

  - Minimizes error over training examples

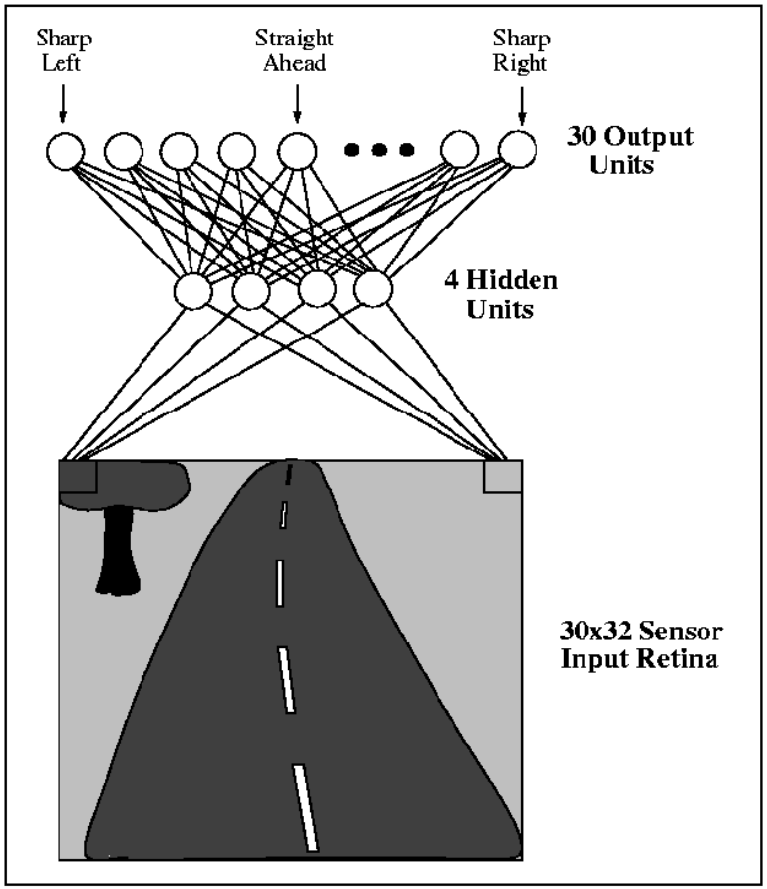
    Generalization to subsequent instances?
  - Training often *very* slow: thousands of iterations over *D* (epochs)
  - Inference (applying network after training) typically very fast
    - Classification
    - Control

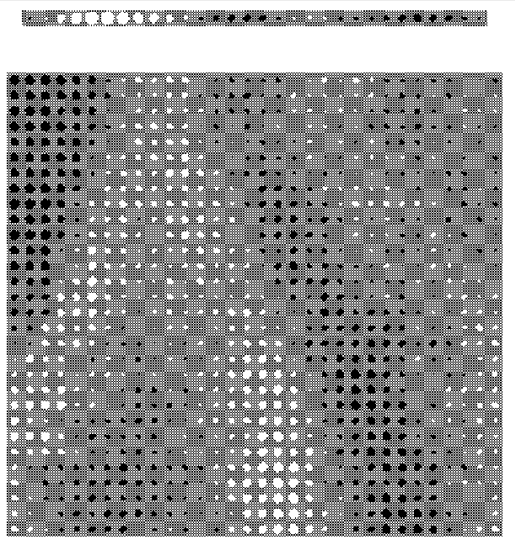
When to Consider Neural Networks

- **Input: High-Dimensional and Discrete or Real-Valued**
  - e.g., raw sensor input
  - Conversion of symbolic data to quantitative (numerical) representations possible
- **Output: Discrete or Real Vector-Valued**
  - e.g., low-level control policy for a robot actuator
  - Similar qualitative/quantitative (symbolic/numerical) conversions may apply
- **Data: Possibly Noisy**
- **Target Function: Unknown Form**
- **Result: Human Readability Less Important Than Performance**
  - Performance measured purely in terms of accuracy and efficiency
  - Readability: ability to explain inferences made using model; similar criteria
- **Examples**
  - Speech phoneme recognition
  - Image classification
  - Financial prediction

Autonomous Learning Vehicle in a Neural Net (ALVINN)

- **Pomerleau *et al***
  - http://www.cs.cmu.edu/afs/cs/project/alv/member/www/projects/ALVINN.html
  - Drives 70mph on highways





Hidden-to-Output Unit Weight Map (for one hidden unit)

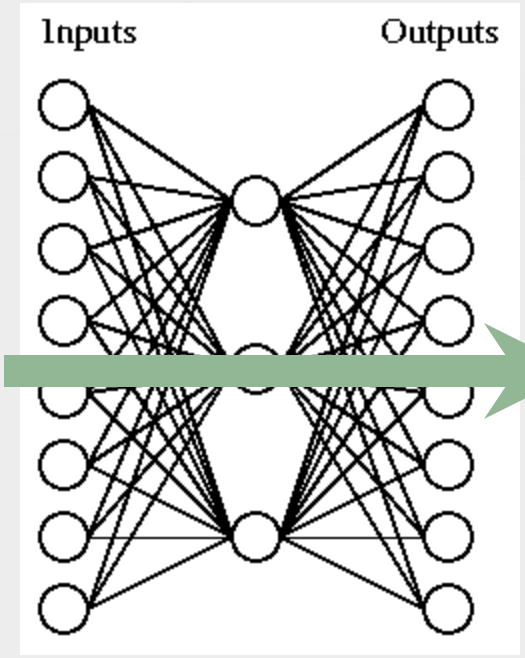
Input-to-Hidden Unit Weight Map (for one hidden unit)

Feedforward ANNs: Representational Power

- **Representational (i.e., Expressive) Power**
  - 2-layer feedforward ANN
    - Any Boolean function
    - Any bounded continuous function (*approximate with arbitrarily small error*) : 1 output (unthresholded linear units) + 1 hidden (sigmoid)
  - 3-layer feedforward ANN: any function (*approximate with arbitrarily small error*): output (linear units), 2 hidden (sigmoid)

Learning Hidden Layer Representations

- **Hidden Units and Feature Extraction**
  - Training procedure: hidden unit representations that minimize error E
  - Sometimes backprop will define new hidden features that are not explicit in the input representation *x*, but which capture properties of the input instances that are most relevant to learning the target function *t*(*x*)
  - Hidden units express *newly constructed features*
  - *Change of representation* to linearly separable *D'*



- **A Target Function (Sparse *aka* 1-of-C, Coding)**

Input									Hidden Values				Output							
1	0	0	0	0	0	0	0	→	0.89	0.04	0.08	→	1	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	→	0.01	0.11	0.88	→	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	→	0.01	0.97	0.27	→	0	0	1	0	0	0	0	0
0	0	0	1	0	0	0	0	→	0.99	0.97	0.71	→	0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0	→	0.03	0.05	0.02	→	0	0	0	0	1	0	0	0
0	0	0	0	0	1	0	0	→	0.22	0.99	0.99	→	0	0	0	0	0	1	0	0
0	0	0	0	0	0	1	0	→	0.80	0.01	0.98	→	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1	→	0.60	0.94	0.01	→	0	0	0	0	0	0	0	1

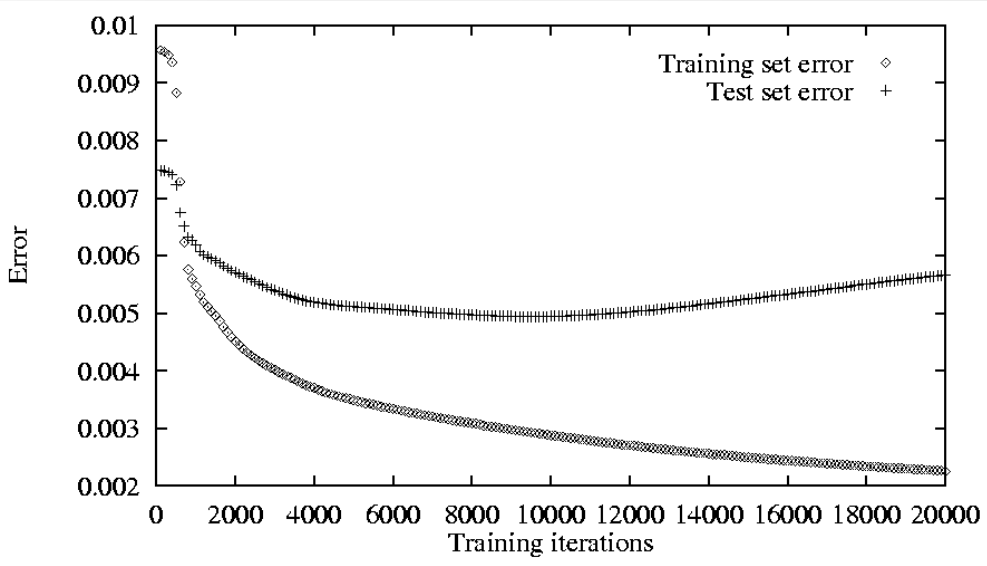
  - ANNs learn discover useful representations at the hidden layers

Convergence of Backpropagation

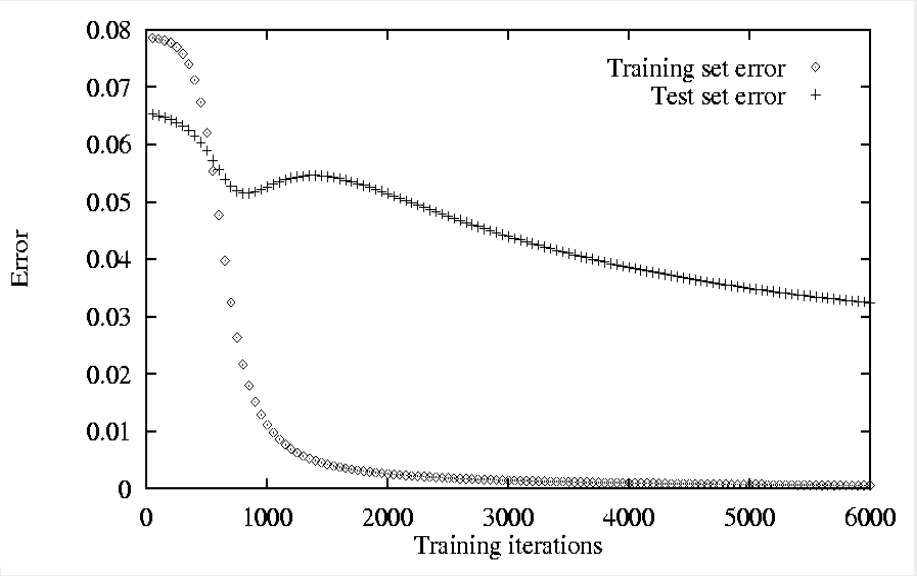
- **No Guarantee of Convergence to Global Optimum**
  - Compare: perceptron convergence (to best $h \in H$, *provided* $h \in H$; i.e., LS)
  - Gradient descent to some local error minimum (perhaps not global)
  - Possible improvements on Backprop (BP) (see later)
    - Momentum term (BP variant; slightly different weight update rule)
    - Stochastic gradient descent (BP variant)
    - Train multiple nets with different initial weights
  - Improvements on feedforward networks
    - Bayesian learning for ANNs
    - Other global optimization methods that integrate over multiple networks

Overtraining in ANNs

- **Recall: Definition of Overfitting**
  - *Performance of the model improves (converges) on* D_{train}, but worsens (or much worse) on D_{test}
- **Overtraining: A Type of Overfitting**
  - *Due to excessive iterations*



Error versus epochs (Example 1)



Error versus epochs (Example 2)

Overfitting in ANNs

- **Other Possible Causes of Overfitting**
  - Number of hidden units sometimes set in advance
  - Too many hidden units ("**overfitting**")
    - The network can memorise to a large extent the specifics of the training data
    - Analogy: fitting a quadratic polynomial with an approximator of degree >> 2
  - Too few hidden units ("**underfitting**")
    - ANNs with no growth
    - Analogy: underdetermined linear system of equations (more unknowns than equations)

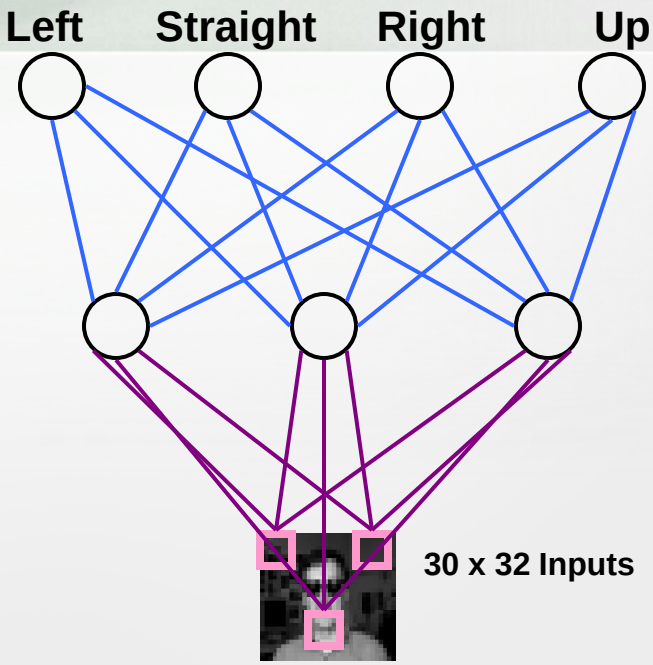
Overfitting in ANNs

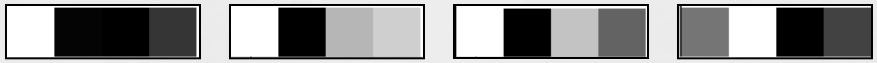
- **Solution Approaches**
  - Prevention: attribute subset selection
  - Avoidance
    - Hold out cross-validation (CV) set or split *k* ways (when to stop?)
    - Weight decay: decrease each weight by some factor on each epoch
  - Detection/recovery: random restarts, addition and deletion of units

Example: Neural Nets for Face Recognition
The Task (http://www.cs.cmu.edu/~tom/faces.html)

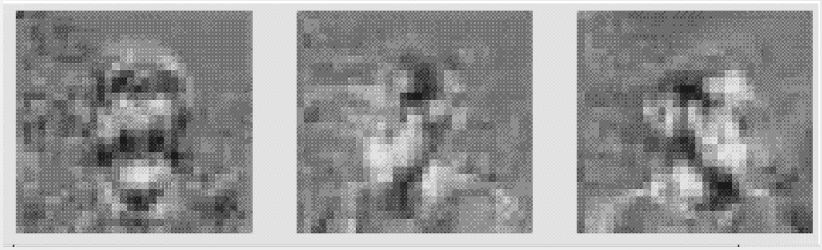
- **Learning Task**: Classifying Camera Images of faces of various people in various poses:
  - 20 people; 32 images per person (624 greyscale images, each with resolution 120 x 128, greyscale intensity 0 (black) to 255 (white))
  - varying expressions (happy, sad, angry, neutral)
  - Varying directions (looking left, right, straight ahead, up)
  - Wearing glasses or not
  - Variation in background behind the person
  - Clothing worn by the person
  - Position of face within image
- **Variety of target functions can be learned**
  - Id of person; direction; gender; wearing glasses; etc.
- **In this case**: learn direction in which person is facing

Neural Nets for Face Recognition

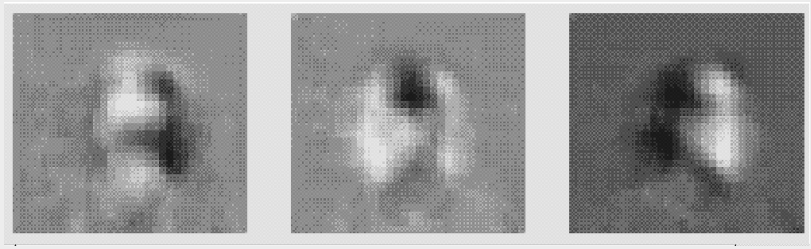




Output Layer Weights (including $w_0 = \theta$) after 1 Epoch



Hidden Layer Weights after 25 Epochs



Hidden Layer Weights after 1 Epoch

- **90% Accurate Learning Head Pose, Recognizing 1-of-20 Faces**

Neural Nets for Face Recognition: Design Choices

- **Input Encoding:**
  - How to encode an image?
    - Extract edges, regions of uniform intensity, other local features?
    - Problem: variable number of features ➔ variable # of input units
  - Choice: encode image as 30 x 32 pixel intensity values (summary/means of original 120 x 128) ➔ computational demands manageable
    - This is crucial in case of ALVINN (autonomous driving)
- **Output Encoding:**
  - ANN to output 1 of 4 values
    - Option1: single unit (values e.g. 0.2, 0.4, 0.6, 0.8)
    - Option2: 1-of-n output encoding (better option)
      - Note: Instead of 0 and 1 values, 0.1 and 0.9 are used (sigmoid units cannot output 0 and 1 given finite weights)

Neural Nets for Face Recognition: Design Choices

- **Network graph structure:** How many units to include and how to interconnect them
  - Commonly: 1 or 2 layers of sigmoid units (occasionally 3). If more, training becomes long!
  - How many hidden units? Fairly small preferable.
    - E.g. with 3 hidden units: 5 min. training; 90%
      with 30 hidden units: 1 hour training; barely better

- **Other Learning Algorithm Parameters:**
  - Learning rate: r = 0.3; momentum α = 0.3 (if too big, training fails to converge with acceptable error)
  - Full gradient descent used.

Neural Nets for Face Recognition: Design Choices

- Network weights
  - Initialised to small random values
- Input unit weights
  - Initialised to zero
- Number of training iterations
  - Data partitioned into training set and validation set
- Gradient descent used
  - Every 50 steps, network performance evaluated over the validation set
  - Final network: the one with highest accuracy over validation set
  - Final result (90%) measured over 3rd set of examples

Example: *NetTalk*

- **Sejnowski and Rosenberg, 1987**
- **Early Large-Scale Application of Backprop**
  - Learning to convert text to speech
    - Acquired model: *a mapping from letters to phonemes and stress marks*
    - Output passed to a speech synthesizer
  - Good performance after training on a vocabulary of ~1000 words
- **Very Sophisticated Input-Output Encoding**
  - Input: 7-letter window; determines the phoneme for the center letter and context on each side; distributed (i.e., sparse) representation: 200 bits
  - Output: units for articulatory modifiers (e.g., “voiced”), stress, closest phoneme; distributed representation
  - 40 hidden units; 10000 weights total
- **Experimental Results**
  - Vocabulary: trained on 1024 of 1463 (informal) and 1000 of 20000 (dictionary)
  - 78% on informal, ~60% on dictionary
- **http://www.boltz.cs.cmu.edu/benchmarks/nettalk.html**

Training (Learning) Functions

- During training: network weights and biases are iteratively adjusted to minimize its Error (/ Loss / performance) function
- Mean Squared Error: default error function for feedforward networks
- Different training algorithms for feedforward networks.
- All are based on the use of the gradient of the error function (to determine how to adjust the weights)
- Gradient determined using backpropagation
- Basic backpropagation training algorithm: weights are updated so as to move in the direction of the negative of the gradient

More on Backpropagation

- One iteration of backpropagation updates the weights as $w_{k+1} = w_k + \alpha_k g_k$
  where at iteration k
  - w_k : vector of weights and biases,
  - g_k : current gradient, and
  - α_k : learning rate.
- Two ways of implementing gradient descent :
  - **incremental mode**: gradient computed and weights updated after each input to the network.
  - **batch mode**: all the inputs are fed into the network before the weights are updated.

Variations of the Backpropagation Algorithm

Batch (Steepest) Gradient Descent training:

- Weights and biases updated in the direction of the negative gradient of the performance function
- The larger the learning rate, the bigger the step.
- If learning rate is set too large, then the algorithm becomes unstable.
- If the learning rate is set too small, the algorithm takes a long time to converge.
- Stopping conditions: max number of iterations, performance gets below the Goal, gradient magnitude smaller than a minimum, maximum training time reached, etc.

Faster Training

- **GD** often too slow for practical problems
- Several high-performance algorithms can converge from 10 to 100 times faster
- The faster algorithms fall into two categories:
  1. Those using heuristic techniques
  2. Those using standard numerical optimization techniques

Faster Algorithms using Heuristic Functions

- GD with momentum
- Adaptive learning rate backpropagation
- Resilient backpropagation

Faster Algorithms using Heuristic Functions

Gradient Descent with Momentum

- Makes the network to respond to the local gradient, **plus** the recent trends in the error surface

$$\Delta w_{start\text{-}layer,end\text{-}layer}(n) = r\,\delta_{end\text{-}layer}\,a_{end\text{-}layer} + \alpha \Delta w_{start\text{-}layer,end\text{-}layer}(n-1)$$

- Two training parameters:
  - Learning rate
  - Momentum:
    - value between 0 (no momentum) and close to 1 (lots of momentum).
    - If momentum = 1 , then network insensitive to the local gradient ➔ does not learn properly.

- Remains quite slow

Faster Algorithms using Heuristic Functions

Adaptive learning rate backpropagation

- With SGD, learning rate is kept constant throughout training. ➔ algorithm performance very sensitive to proper setting of learning rate.
- If *lr* is too large, the algorithm can oscillate and become unstable.
- If *lr* is too small, the algorithm takes too long to converge.
- Possible to improve the performance of SGD by allowing the learning rate to change during training.
- Adaptive learning rate attempts to keep the learning step size as large as possible while keeping learning stable.
- Learning rate is made responsive to the complexity of the local error surface.

Adaptive learning rate backpropagation (cont.)

- If new error exceeds the old error by more than a predefined ratio (typically 1.04),
  - the new weights and biases are discarded.
  - The learning rate is decreased (typically multiplying by a factor of 0.7).

  Otherwise, the new weights and biases, are kept.
- If new error less than old error, the learning rate is increased (typically multiplying by a factor 1.05).
- A near-optimal learning rate can be obtained for the given problem
- One can combine Adaptive learning rate with Momentum

Faster Algorithms using Heuristic Functions

Resilient Backpropagation:

Problem with Sigmoid functions: their slopes approach zero as the input gets large

➔ the gradient can have a very small magnitude

➔ small changes in weights and biases, even though the weights and biases are far from their optimal values.

- Resilient backpropagation attempts to eliminate harmful effects of the magnitudes of the gradient
- Magnitude of the gradient has no effect on the weight update
- Only the sign of the gradient is used to determine the direction of the weight update;

Resilient Backpropagation (cont.)

- The size of weight change is determined by a separate update value.
- The update value for each weight and bias is increased by a factor *delt_inc* whenever the derivative of the performance function with respect to that weight has the same sign for two successive iterations.
- The update value is decreased by a factor *delt_dec* whenever the derivative with respect to that weight changes sign from the previous iteration.
- If the derivative is zero, then the update value remains the same.
- So: Whenever the weights are oscillating, the weight change is reduced.
- If the weight continues to change in the same direction for several iterations, then the magnitude of the weight change increases.

Resilient Backpropagation (cont.)

- Generally much faster than the standard steepest descent algorithm.
- Requires only a modest increase in memory requirements

Faster Algorithms using Standard Numerical Optimization Techniques

- **Conjugate Gradient Algorithms**
- Basic Backpropagation algorithm adjusts the weights in the steepest descent direction (negative of the gradient), the direction in which the performance function is decreasing most rapidly.
- This does not necessarily produce the fastest convergence.
- In **conjugate gradient algorithms** a search is performed along conjugate directions, which produces generally faster convergence than steepest descent directions.
- In most of conjugate gradient algorithms, the step size is adjusted at each iteration.
- A search is made along the conjugate gradient direction to determine the step size that minimizes the performance function along that line

Conjugate Gradient Algorithms

- Fletcher-Reeves Update
- Polak-Ribiére Update
- Powell-Beale Restarts
- Scaled Conjugate Gradient

Conjugate Gradient Algorithms

- All the CG algorithms start by searching in the SGD direction on the first iteration.

$$P_o = - g_o$$

- A line search is then performed to determine the optimal distance to move along the current search direction:

$$x_{k+1} = x_k + \alpha_k P_k$$

- The next search direction is determined so that it is conjugate to previous search directions.
- The general procedure for determining the new search direction is to combine the new steepest descent direction with the previous search direction:

$$p_k = - g_k + \beta_k p_{k-1}$$

Conjugate Gradient Algorithms

- The various versions of the conjugate gradient algorithm are distinguished by the way in which the constant β_k is computed.
- For the **Fletcher-Reeves** update the procedure is

$$\beta_k = \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}}$$

- For the **Polak-Ribiére** update, the constant k is computed by

$$\beta_k = \frac{\Delta g_{k-1}^T g_k}{g_{k-1}^T g_{k-1}}$$

- Etc.

Faster Algorithms using Standard Numerical Optimization Techniques

- **Quasi-Newton Algorithms**
- Basic step of Newton's method is

$$X_{k+1} = -X_k + A_k^{-1} g_k$$

where A_k^{-1} is the Hessian matrix (second derivatives) of the performance.

- Newton's method often converges faster than conjugate gradient methods.
- Computing the Hessian matrix for feedforward neural networks is complex and expensive.
- A class of algorithms that is based on Newton's method, but which doesn't require calculation of second derivatives.
- These are called quasi-Newton (or secant) methods. They update an approximate Hessian matrix at each iteration of the algorithm.

Some ANN Applications

- **Diagnosis**
  - Closest to pure concept learning and classification
  - Some ANNs can be post-processed to produce probabilistic diagnoses
- **Prediction and Monitoring**
  - *aka* prognosis (sometimes forecasting)
  - Predict a continuation of (typically numerical) data
- **Decision Support Systems**
  - *aka* recommender systems
  - Provide assistance to human "subject matter" experts in making decisions
    - Design (manufacturing, engineering)
    - Therapy (medicine)
    - Crisis management (medical, economic, military, computer security)
- **Control Automation**
  - Mobile robots
  - Autonomic sensors and actuators
- **Many, Many More**

Strengths of a Neural Network

- **Power**: Model complex functions, nonlinearity built into the network
- **Ease of use**:
  - Learn by example
  - Very little user domain-specific expertise needed
- **Intuitively appealing**: based on model of biology, will it lead to genuinely intelligent computers/robots?

General Advantages / Disadvantages

- **Advantages**
  - Adapt to unknown situations
  - Robustness: fault tolerance due to network redundancy
  - Autonomous learning and generalization

- **Disadvantages**
  - Complexity of finding the “right” network structure
  - “Black box”

Issues and Open Problems in (classical) ANN Research

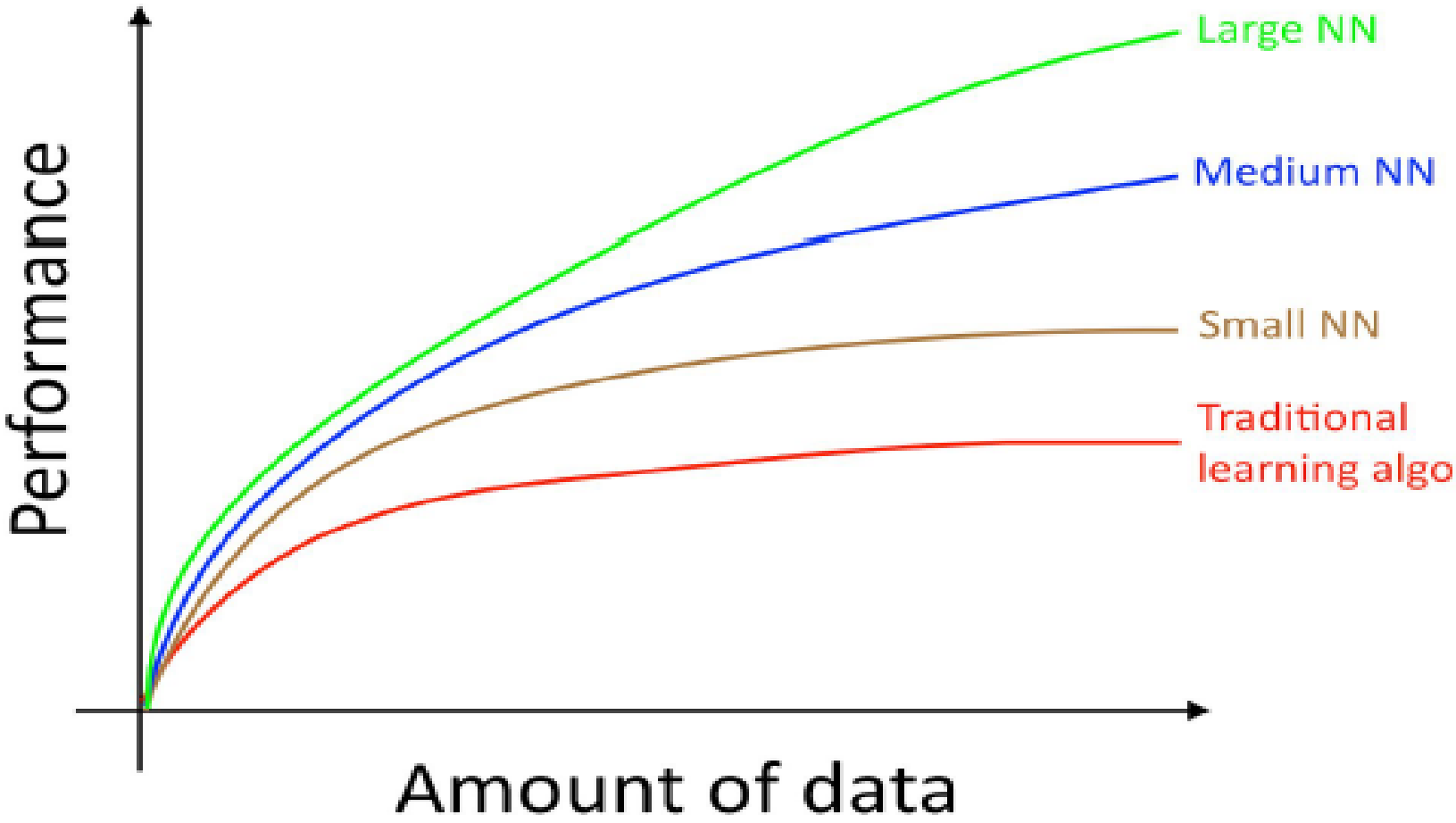
- **Hybrid Approaches**
  - Incorporating knowledge and analytical learning into ANNs
    - Knowledge-based neural networks
    - Explanation-based neural networks
    - Combining uncertain reasoning and ANN learning and inference
    - Probabilistic ANNs
    - Bayesian networks

Issues and Open Problems in (classical) ANN Research

- **Global Optimization with ANNs**
  - Hybrid models
  - Relationship to genetic algorithms
- **Understanding ANN Output**
  - Knowledge extraction from ANNs
    - Rule extraction
    - Other decision surfaces
  - Decision support and KDD applications
- **Many More Issues (Robust Reasoning, Representations, etc.)**

Going Deep?

Andrew Ng, Machine Learning Yearning, --Technical Strategy for AI Engineers in the Era of Deep Learning, Draft Version, 2018, deeplearning.ai



This presentation was based on the following:

- *Tom Mitchell*, *Machine Learning*, McGraw Hill, 1997
- Lecture notes by Prof. Hsu (Kansas State University) based on Tom Mitchell's Machine Learning book.
- Training Functions and Fast Training, Matlab documentation, Mathworks.
- Andrew Ng, Machine Learning and Deep Learning online course, Coursera.
- Dave Touretzki, « Artificial Neural Networks » Lecture notes, Carnegie Mellon University, http://www.cs.cmu.edu/afs/cs.cmu.edu/academic/class/15782-f06/syllabus.html
- Nicolas Galoppo von Borries, Introduction to Neural Networks, COMP290-058 Motion Planning. (http://slideplayer.com/slide/9882811/)

Thank you!