

Lecture 13 of 42

AMA-Talk - Yihao group

Multilayer Perceptrons and Intro to Support Vector Machines

- 1. Computer role-playing game
- 2. Multi-agent "game"
- 3. Bioinformatics Learning w/ doc. log₂ BK

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www.kddresearch.org/Courses/Spring-2007/CIS732/

Readings:

- Sections 4.1-4.4, Mitchell
- Section 2.2.6, Shavlik and Dietterich (Rosenblatt)
- Section 2.4.5, Shavlik and Dietterich (Minsky and Papert)



Winnow: Mistake Bound

• Claim: Train-Winnow makes $O(k \log n)$ mistakes on k -disjunctions ($\leq k$ of n)

• Proof

- u = number of mistakes on positive examples (promotions)
- v = number of mistakes on negative examples (demotions/eliminations)

- Lemma 1: $u < k \lg(2n) = k(\lg n + 1) = k \lg n + k = O(k \log n)$

- Proof

- A weight that corresponds to a good variable is only promoted
- When these weights reach n there will be no more false positives

- Lemma 2: $v < 2(u + 1)$

- Proof

- Total weight $W = n$ initially
- False positive: $W(t+1) < W(t) + n$ - in worst case, every variable promoted
- False negative: $W(t+1) < W(t) - n/2$ - elimination of a bad variable
- $0 < W < n + un - vn/2 \Rightarrow v < 2(u + 1)$

- Number of mistakes: $u + v < 3u + 2 = O(k \log n)$, Q.E.D.

Handwritten notes and diagrams:

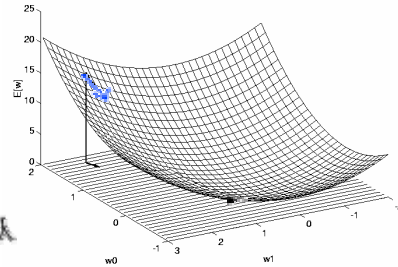
- DNF: $S = x_1 \vee x_2 \vee \dots \vee x_n$
- class $C = x_1 \vee x_2 \vee \dots \vee x_n$
- $F = O(g)$
- $v < 2(u + 1)$
- $f(n) = a g(n)$
- Diagram showing a graph with axes n and W , and curves for $f(n)$ and $g(n)$.
- Diagram showing a tree structure with nodes labeled "initial", "promote", and "demote".
- Diagram showing a list of variables x_1, x_2, \dots, x_n with weights w_1, w_2, \dots, w_n and a threshold n .



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

- **Definition: Gradient**

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



- **Modified Gradient Descent Training Rule**

Sum Squared Error

$$\Delta \bar{w} = -r \nabla E[\bar{w}]$$

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

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

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

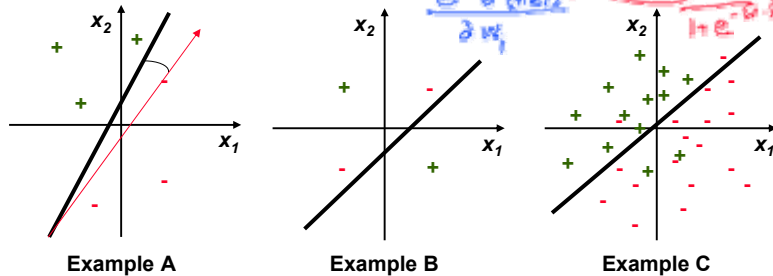
$$\frac{\partial E}{\partial w_i} = \sum_{x \in D} [(t(x) - o(x))(-x_i)]$$

Sgn($\bar{w} \cdot \bar{x}$)

Gradient Descent: Algorithm using Delta/LMS Rule


- **Algorithm Gradient-Descent (D, r)**
 - Each training example is a pair of the form $\langle x, t(x) \rangle$, where x is the vector of input values and $t(x)$ is the output value. r is the learning rate (e.g., 0.05)
 - Initialize all weights w_i to (small) random values
 - UNTIL the termination condition is met, DO
 - Initialize each Δw_i to zero
 - FOR each $\langle x, t(x) \rangle$ in D , DO
 - Input the instance x to the unit and compute the 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
- **Mechanics of Delta Rule**
 - Gradient is based on a derivative
 - Significance: later, will use nonlinear activation functions (aka transfer functions, squashing functions)

Gradient Descent: Perceptron Rule versus Delta/LMS Rule



- **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
- **Weight Vector w = Sum of Misclassified $x \in D$**
 - Perceptron: minimize w
 - Delta Rule: minimize error \equiv distance from separator (i.e., maximize $\frac{\partial E}{\partial \bar{w}}$)

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Incremental (Stochastic) Gradient Descent

- **Batch Mode Gradient Descent**
 - UNTIL the termination condition is met, DO
 1. Compute the gradient $\nabla E_D[\bar{w}]$
 2. $\bar{w} \leftarrow \bar{w} - r \nabla E_D[\bar{w}]$
 - RETURN final w
- **Incremental (Online) Mode Gradient Descent**
 - UNTIL the termination condition is met, DO
 - FOR each $\langle x, t(x) \rangle$ in D , DO
 1. Compute the gradient $\nabla E_d[\bar{w}]$
 2. $\bar{w} \leftarrow \bar{w} - r \nabla E_d[\bar{w}]$
 - RETURN final w
- **Emulating Batch Mode**
 - $E_D[\bar{w}] \equiv \frac{1}{2} \left[\sum_{x \in D} (t(x) - o(x))^2 \right]$, $E_d[\bar{w}] \equiv \frac{1}{2} (t(x) - o(x))^2$
 - Incremental gradient descent can approximate batch gradient descent arbitrarily closely if r made small enough

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Learning Disjunctions

- **Hidden Disjunction to Be Learned**
 - $c(x) = x_1^{t_1} \vee x_2^{t_2} \vee \dots \vee x_m^{t_m}$ (e.g., $x_2 \vee x_4 \vee x_5 \dots \vee x_{100}$)
 - Number of disjunctions: 3^n (each x_i : included, negation included, or excluded)
 - *Change of representation*: can turn into a monotone disjunctive formula?
 - How?
 - How many disjunctions then?
 - Recall from COLT: mistake bounds
 - $\log(|C|) = O(n)$
 - Elimination algorithm makes $O(n)$ mistakes
- **Many Irrelevant Attributes**
 - Suppose only $k \ll n$ attributes occur in disjunction c - i.e., $\log(|C|) = O(k \log n)$
 - Example: learning natural language (e.g., learning over text)
 - Idea: use a **Winnow** - perceptron-type LTU model (Littlestone, 1988)
 - Strengthen weights for false positives
 - Learn from negative examples too: weaken weights for false negatives

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Winnow Algorithm

- **Algorithm *Train-Winnow* (D)**
 - Initialize: $\theta = n, w_i = 1$
 - UNTIL the termination condition is met, DO
 - FOR each $\langle x, t(x) \rangle$ in D , DO
 1. CASE 1: no mistake - do nothing
 2. CASE 2: $t(x) = 1$ but $w \cdot x < \theta - w_i \leftarrow 2w_i$ if $x_i = 1$ (promotion/strengthening)
 3. CASE 3: $t(x) = 0$ but $w \cdot x \geq \theta - w_i \leftarrow w_i / 2$ if $x_i = 1$ (demotion/weakening)
 - RETURN final w
- **Winnow Algorithm Learns Linear Threshold (LT) Functions**
- **Converting to Disjunction Learning**
 - Replace demotion with elimination
 - Change weight values to 0 instead of halving
 - Why does this work?

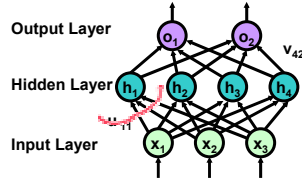
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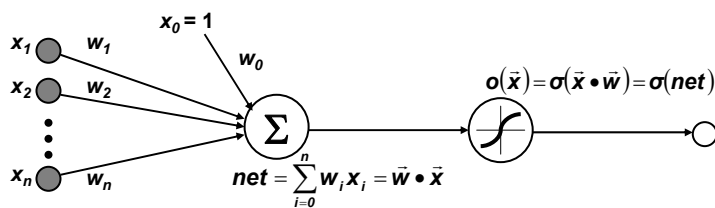


Multi-Layer Networks of Nonlinear Units

- Nonlinear Units** $h_j(x) = \sigma(\vec{a}_j \cdot \vec{x})$
 - Recall: activation function $sgn(w \cdot x)$
 - 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
 - “Layers”: counted in weight layers (e.g., 1 hidden layer = 2-layer network)
 - Only hidden and output layers contain perceptrons (threshold or 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

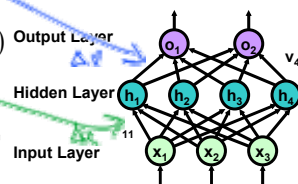


- Sigmoid Activation Function**
 - Linear threshold gate activation function: $sgn(w \cdot x)$
 - Nonlinear activation (aka transfer, squashing) function: generalization of sgn
 - σ is the sigmoid function $\sigma(net) = \frac{1}{1 + e^{-net}}$
 - Can derive gradient rules to train
 - One sigmoid unit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



Backpropagation Algorithm

- **Intuitive Idea: Distribute *Blame* for Error to Previous Layers**
- **Algorithm *Train-by-Backprop* (D, r)**
 - Each training example is a pair of the form $\langle x, t(x) \rangle$, where x is the vector of input values and $t(x)$ is the output value. r is the learning rate (e.g., 0.05)
 - 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 $o(x) = \sigma(\text{net}(x))$
 - FOR each output unit k , DO
 - $\delta_k = o_k(x)(1 - o_k(x))(t_k(x) - o_k(x))$
 - FOR each hidden unit j , DO
 - $\delta_j = h_j(x)(1 - h_j(x)) \sum_{k \in \text{outputs}} v_{j,k} \delta_k$
 - Update each $w = u_{i,j}$ ($a = h_j$) or $w = v_{j,k}$ ($a = o_k$)
 - $w_{\text{start-layer, end-layer}} \leftarrow w_{\text{start-layer, end-layer}} + \Delta w_{\text{start-layer, end-layer}}$
 - $\Delta w_{\text{start-layer, end-layer}} \leftarrow r \delta_{\text{end-layer}} a_{\text{end-layer}}$
 - RETURN final u, v

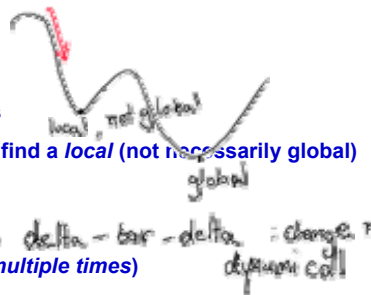


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Backpropagation and Local Optima

- **Gradient Descent in Backprop**
 - Performed over entire *network* weight vector
 - Easily generalized to arbitrary directed graphs
 - Property: Backprop on feedforward ANNs will find a *local* (not necessarily global) error minimum
- **Backprop in Practice**
 - Local optimization often works well (can run *multiple times*)
 - Often include weight momentum $\alpha \in [0, 1]$
 - $\Delta w_{\text{start-layer, end-layer}}(n) = r \delta_{\text{end-layer}} a_{\text{end-layer}} + \alpha \Delta w_{\text{start-layer, end-layer}}(n-1)$
 - 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



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Feedforward ANNs: Representational Power and Bias

- **Representational (i.e., Expressive) Power** *f.e. small enough*
 - Backprop presented for feedforward ANNs with single hidden layer (2-layer)
 - 2-layer feedforward ANN
 - Any **Boolean function** (simulate a 2-layer AND-OR network) *large enough*
 - Any **bounded continuous function** (*approximate with arbitrarily small error*) [Cybenko, 1989; Hornik *et al*, 1989]
 - Sigmoid functions: set of **basis functions**; used to compose arbitrary functions
 - 3-layer feedforward ANN: any function (*approximate with arbitrarily small error*) [Cybenko, 1988]
 - Functions that ANNs are good at acquiring: **Network Efficiently Representable Functions (NERFs)** - how to characterize? [Russell and Norvig, 1995]
- **Inductive Bias of ANNs**
 - n -dimensional Euclidean space (**weight space**)
 - Continuous (error function smooth with respect to weight parameters)
 - Preference bias: “smooth interpolation” among positive examples
 - Not well understood yet (known to be computationally hard)



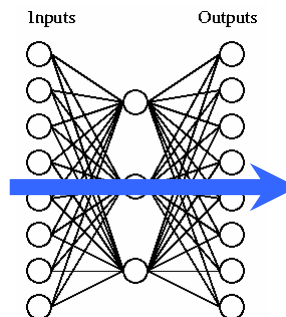
Learning Hidden Layer Representations

- **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'*

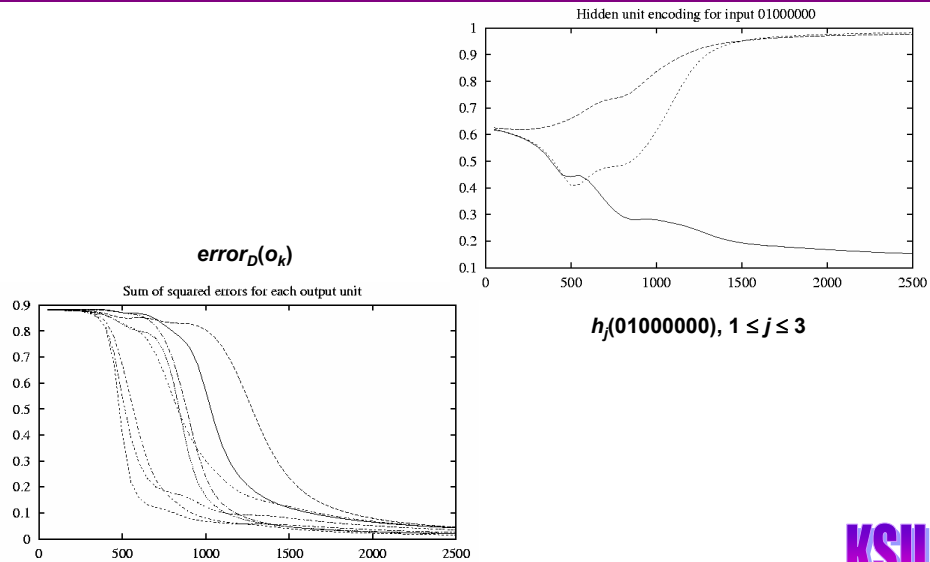
- **A Target Function (Sparse aka 1-of-C, Coding)**

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

- Can this be learned? (Why or why not?)



Training: Evolution of Error and Hidden Unit Encoding

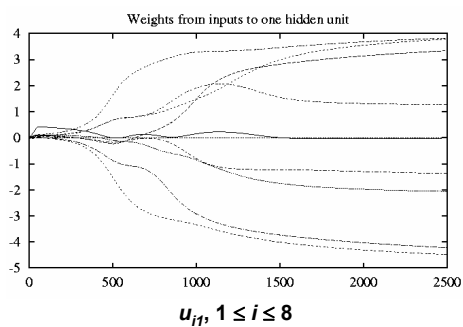


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Training: Weight Evolution



- **Input-to-Hidden Unit Weights and Feature Extraction**
 - Changes in first weight layer values correspond to changes in hidden layer encoding and consequent output squared errors
 - w_0 (bias weight, analogue of threshold in LTU) converges to a value near 0
 - Several changes in first 1000 epochs (different encodings)

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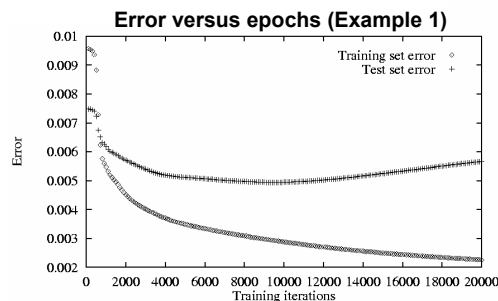
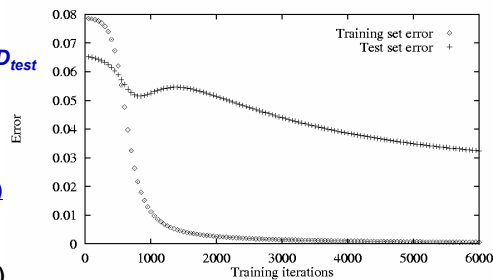
Convergence of Backpropagation

- **No Guarantee of Convergence to Global Optimum Solution**
 - 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 minimum...)
 - Possible improvements on backprop (BP)
 - Momentum term (BP variant with slightly different weight update rule)
 - Stochastic gradient descent (BP algorithm variant)
 - Train multiple nets with different initial weights; find a good mixture
 - Improvements on feedforward networks
 - Bayesian learning for ANNs (e.g., simulated annealing) - later
 - Other global optimization methods that integrate over multiple networks
- **Nature of Convergence**
 - Initialize weights near zero
 - Therefore, initial network near-linear
 - Increasingly non-linear functions possible as training progresses



Overtraining in ANNs

- **Recall: Definition of Overfitting**
 - h' worse than h on D_{train} , better on D_{test}
- **Overtraining: A Type of Overfitting**
 - Due to excessive iterations
 - **Avoidance: stopping criterion**
(cross-validation: holdout, k-fold)
 - **Avoidance: weight decay**



Error versus epochs (Example 2)



Overfitting in ANNs

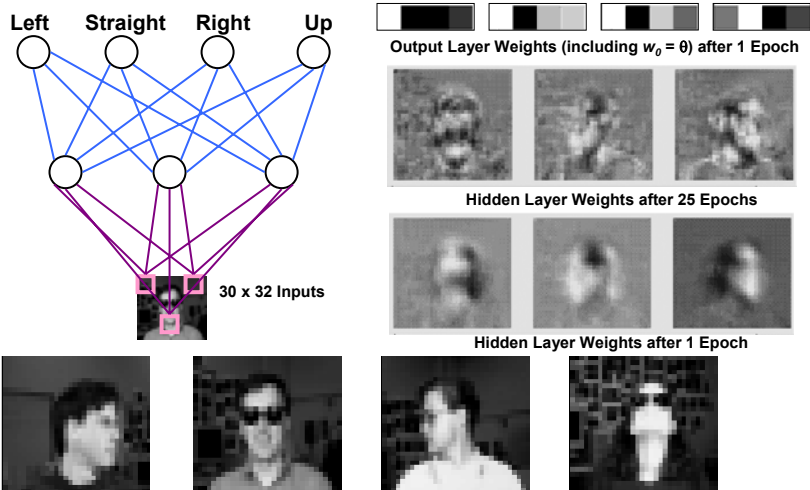
- **Other Causes of Overfitting Possible**
 - Number of hidden units sometimes set in advance
 - Too few hidden units (“underfitting”)
 - ANNs with no growth
 - Analogy: underdetermined linear system of equations (more unknowns than equations)
 - Too many hidden units
 - ANNs with no pruning
 - Analogy: fitting a quadratic polynomial with an approximator of degree $\gg 2$
- **Solution Approaches**
 - Prevention: attribute subset selection (using pre-filter or wrapper)
 - 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 weights, units



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Example: Neural Nets for Face Recognition



- **90% Accurate Learning Head Pose, Recognizing 1-of-20 Faces**
- <http://www.cs.cmu.edu/~tom/faces.html>



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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>



Alternative Error Functions

- Penalize Large Weights (with Penalty Factor w_p)

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{\langle \vec{x}, t(\vec{x}) \rangle \in D} \sum_{k \in \text{outputs}} \left[(t_k(\vec{x}) - o_k(\vec{x}))^2 + w_p \sum_{\text{start-layer, end-layer}} w^2 \right]$$

- Train on Both Target Slopes and Values

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{\langle \vec{x}, t(\vec{x}) \rangle \in D} \sum_{k \in \text{outputs}} \left[(t_k(\vec{x}) - o_k(\vec{x}))^2 + w_s \sum_{i \in \text{inputs}} \left(\frac{\partial t_k(\vec{x})}{\partial x_i} - \frac{\partial o_k(\vec{x})}{\partial x_i} \right)^2 \right]$$

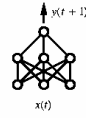
- Tie Together Weights

- e.g., in phoneme recognition network
- See: *Connectionist Speech Recognition* [Bourlard and Morgan, 1994]

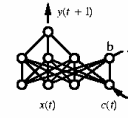


Recurrent Networks

- **Representing Time Series with ANNs**
 - Feedforward ANN: $y(t + 1) = \text{net}(x(t))$
 - Need to capture temporal relationships



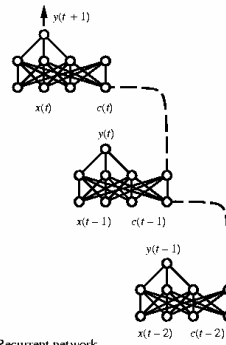
(a) Feedforward network



(b) Recurrent network

- **Solution Approaches**

- Directed cycles
- Feedback
 - Output-to-input [Jordan]
 - Hidden-to-input [Elman]
 - Input-to-input
- Captures **time-lagged relationships**
 - Among $x(t' \leq t)$ and $y(t + 1)$
 - Among $y(t' \leq t)$ and $y(t + 1)$
- Learning with recurrent ANNs
 - Elman, 1990; Jordan, 1987
 - Principe and deVries, 1992
 - Mozer, 1994; Hsu and Ray, 1998



(c) Recurrent network unfolded in time



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New Neuronal Models

- **Neurons with State**
 - **Neuroids** [Valiant, 1994]
 - Each basic unit may have a state
 - Each may use a different update rule (or compute differently based on state)
 - Adaptive model of network
 - Random graph structure
 - Basic elements receive meaning as part of learning process
- **Pulse Coding**
 - Spiking neurons [Maass and Schmitt, 1997]
 - Output represents more than activation level
 - Phase shift between firing sequences counts and adds expressivity
- **New Update Rules**
 - Non-additive update [Stein and Meredith, 1993; Seguin, 1998]
 - Spiking neuron model
- **Other Temporal Codings: (Firing) Rate Coding**



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Some Current Issues and Open Problems in ANN Research

- **Hybrid Approaches**
 - Incorporating knowledge and analytical learning into ANNs
 - Knowledge-based neural networks [Flann and Dietterich, 1989]
 - Explanation-based neural networks [Towell *et al*, 1990; Thrun, 1996]
 - Combining uncertain reasoning and ANN learning and inference
 - Probabilistic ANNs
 - Bayesian networks [Pearl, 1988; Heckerman, 1996; Hinton *et al*, 1997] - later
- **Global Optimization with ANNs**
 - Markov chain Monte Carlo (MCMC) [Neal, 1996] - e.g., simulated annealing
 - Relationship to genetic algorithms - later
- **Understanding ANN Output**
 - Knowledge extraction from ANNs
 - Rule extraction
 - Other decision surfaces
 - Decision support and KDD applications [Fayyad *et al*, 1996]
- **Many, Many More Issues (Robust Reasoning, Representations, etc.)**



Term Project Topics



Terminology

- **Multi-Layer ANNs**
 - Focused on one species: (feedforward) multi-layer perceptrons (MLPs)
 - Input layer: an implicit layer containing x_i
 - Hidden layer: a layer containing input-to-hidden unit weights and producing h_j
 - Output layer: a layer containing hidden-to-output unit weights and producing o_k
 - n-layer ANN: an ANN containing $n - 1$ hidden layers
 - Epoch: one training iteration
 - Basis function: set of functions that span H
- **Overfitting**
 - Overfitting: h does better than h' on training data and worse on test data
 - Overtraining: overfitting due to training for too many epochs
 - Prevention, avoidance, and recovery techniques
 - Prevention: attribute subset selection
 - Avoidance: stopping (termination) criteria (CV-based), weight decay
- **Recurrent ANNs: Temporal ANNs with Directed Cycles**



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Summary Points

- **Multi-Layer ANNs**
 - Focused on feedforward MLPs
 - Backpropagation of error: distributes penalty (loss) function throughout network
 - Gradient learning: takes derivative of error surface with respect to weights
 - Error is based on difference between desired output (t) and actual output (o)
 - Actual output (o) is based on activation function
 - Must take partial derivative of $\sigma \Rightarrow$ choose one that is easy to differentiate
 - Two σ definitions: sigmoid (aka logistic) and hyperbolic tangent (\tanh)
- **Overfitting in ANNs**
 - Prevention: attribute subset selection
 - Avoidance: cross-validation, weight decay
- **ANN Applications: Face Recognition, Text-to-Speech**
- **Open Problems**
- **Recurrent ANNs: Can Express Temporal Depth (Non-Markovity)**
- **Next: Statistical Foundations and Evaluation, Bayesian Learning Intro**



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