Artificial Neural Networks (ANN)

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Computer Science 760

Artificial Neural Networks

- Robust approach to approximating real-valued, discrete-valued, and vector-valued target functions
- For certain types of problems (complex real-world sensor data), ANN are the most effective learning methods currently known
- Learning to recognise handwritten characters, spoken words, or faces

Inspiration

- Biological learning systems are built of very complex webs of interconnected neurons
- ANNs are built of a densely interconnected set of simple units, where each unit takes a number of real-valued inputs (possibly the outputs of other units) and produces a single real-valued output (which may become the input to many other units)

Human Brain

- 10^{11} densely interconnected neurons
- Each neuron connected to 10^{4} others
- Switching time:
  - Human 10^{-3} seconds
  - Computer 10^{-4} seconds
- 10^{-1} seconds to visually recognise your mother, so only a few hundred steps
- Must be highly parallel computation based on distributed representations

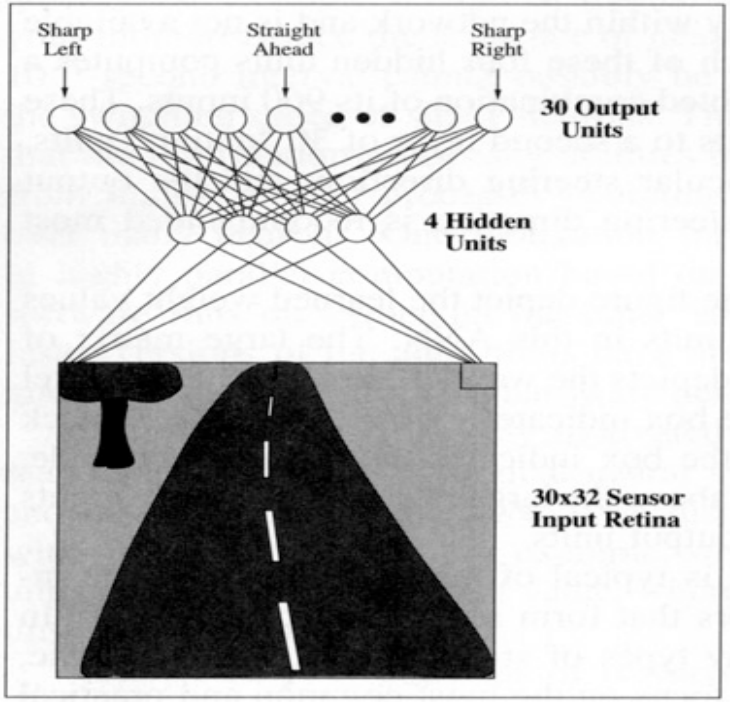
Researchers

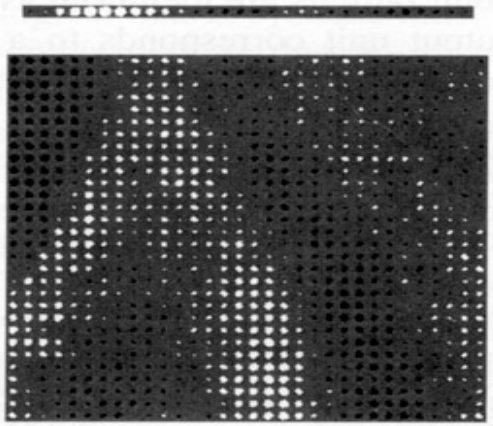
- Two Groups of Researchers:
  - Use ANN to study and model biological learning processes
  - Obtaining highly effective machine learning algorithms

Neural Network Representations

- ALVINN - ANN to steer an autonomous vehicle driving at normal speeds on public highways
- Input - 30 x 32 grid of pixel intensities from a forward-pointed camera
- Output - direction vehicle is steered
- Trained to mimic the observed steering commands of a human driving the vehicle for 5 minutes

ALVINN's ANN


Sharp Left
Straight Ahead
Sharp Right
30 Output Units
4 Hidden Units
30x32 Sensor Input Retina



Backpropagation Network Representations

- Individual units interconnected in layers that form a directed graph
- Learning corresponds to choosing a weight value for each edge in the graph
- Certain types of cycles are allowed
- Vast majority of practical applications are acyclic feed-forward networks like ALVINN

Appropriate Problems for ANN

- Training data is noisy, complex sensor data
- Also problems where symbolic algorithms are used (decision tree learning (DTL)) - ANN and DTL produce results of comparable accuracy

Specifically

- Instances are attribute-value pairs, attributes may be highly correlated or independent, values can be any real value
- Target function may be discrete-valued, real-valued or vector-valued
- Training examples may contain errors
- Long training times are acceptable
- Can Require fast evaluation of the learned target function
- Humans do NOT need to understand the learned target function

Perceptrons

- Inputs a vector of real-valued inputs calculates a linear combination and outputs a 1 if the result is greater than some threshold and -1 otherwise
- Hyperplane decision surface in the n-dimensional space of instances
- Not all datasets can be separated by a hyperplane, but if they can they are ***linearly separable*** datasets

Linearly Separable

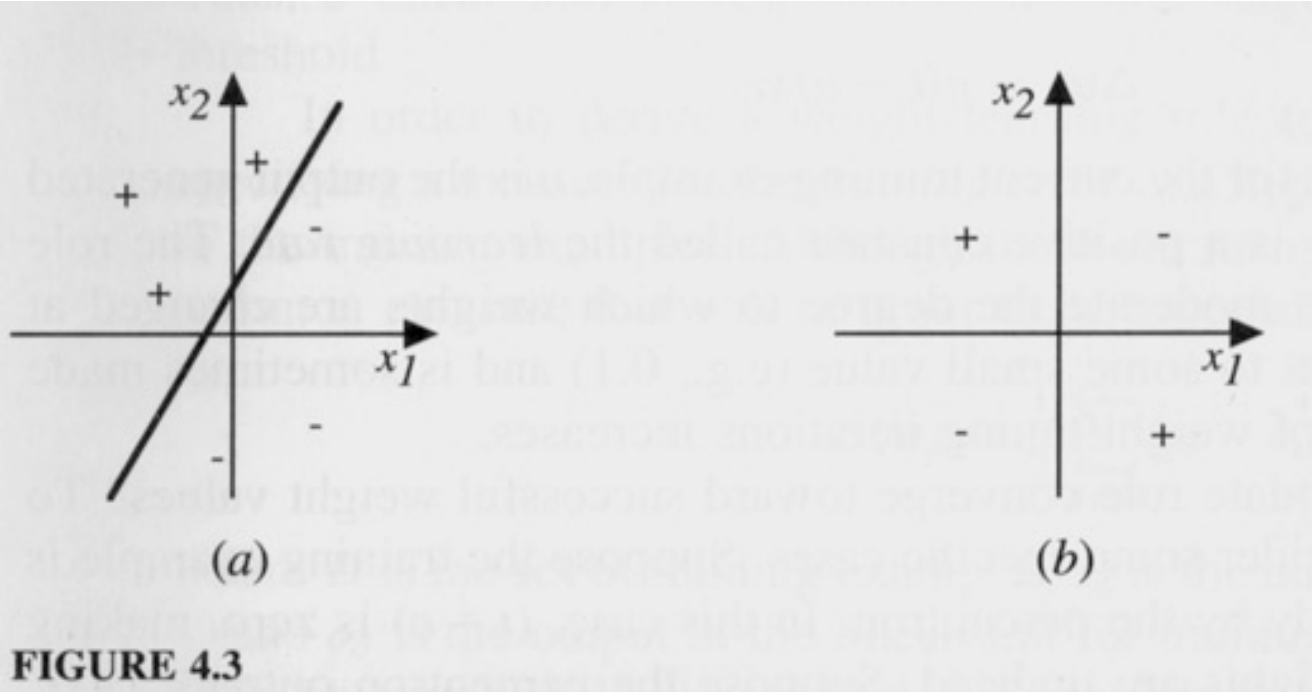


FIGURE 4.3

Specifically

$$o(x1,..,xn) = 1 \quad if\ w_0 + w_1 x_1 + w_2 x_2 + ... + w_n x_n > 0$$
$$= -1 \quad otherwise$$

- Each w_i is a real-valued weight that determines the contribution of the input x_i to the perceptron output
- The quantity ($-w_0$) is the threshold

A Perceptron

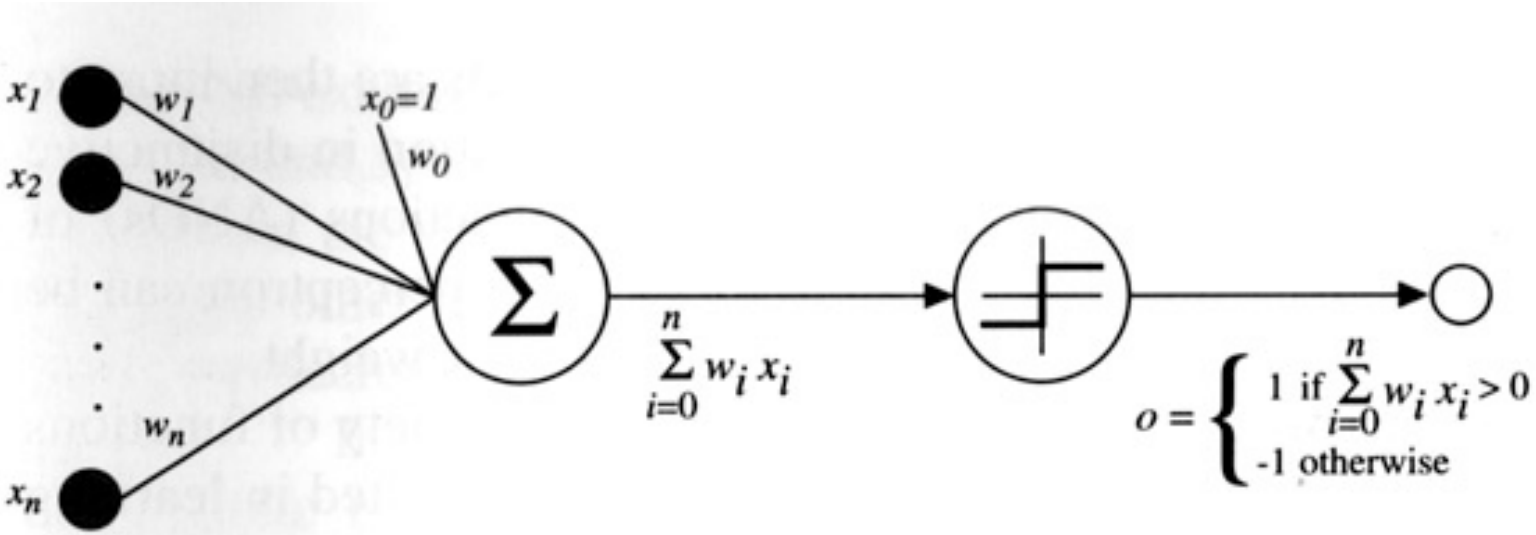


FIGURE 4.2
A perceptron.

Representational Power of Perceptrons

- A single perceptron can represent many boolean functions
- If 1 (true) and -1 (false), then to implement an AND function make $w_0 = -0.8$ and $w_1 = w_2 = 0.5$
- A perceptron can represent AND, OR, NAND, and NOR but not XOR!!
- ***Every*** boolean function can be represented by some network of perceptrons only two levels deep

Perceptron Learning Algorithms

- Determine a weight vector that causes the perceptron to produce the correct ±1 output for each of the given training examples
- Several algorithms are known to solve this problem:
  - the perceptron rule
  - The delta rule
- Guaranteed to converge to somewhat different acceptable hypothesis under somewhat different conditions
- These are the basis for learning networks of many units - ANNs

Perceptron Training Rule

- Begin with random weights, modify them, repeat until the perceptron classifies all training examples correctly
- ***Perceptron rule:***

$$w_i \leftarrow w_i + \Delta w_i, \; where \; \Delta w_i = \eta\left(t - o\right)x_i$$

- ***t*** is the target output, ***o*** is the output generated by the perceptron, and ***η*** is the ***learning rate*** which moderates the degree to which weights are changed at each step, usually set to a small value (0.1)

Intuition for Perceptron Training Rule

- If the training example is correctly classified

  (t-o)=0, making $\Delta w_i = 0$, so no weights are updated
- If the perceptron outputs -1 when the target output is +1 and assuming $\eta = 0.1$ and $x_i = 0.8$, then $\Delta w_i = 0.1(1-(-1))0.8 = 0.16$
- If the perceptron outputs +1 when the target output is -1, then the weight would be decreased

Convergence of Perceptron Training Rule

- This learning procedure will converge within ***finite*** number of applications of the perceptron training rule to a weight vector that correctly classifies all training examples, ***provided the training examples are linearly separable*** and a sufficiently small η is used.

Gradient Descent Algorithm

- If training examples are not linearly separable, the delta rule converges toward best-fit approximation
- Use ***gradient descent*** to find the weights that best fit the training examples - basis of the Backpropagation Algorithm

Error Definition

- Assume an unthresholded perceptron, then the training error is

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

- Where ***D*** is the set of training examples $\boldsymbol{t_d}$ is the target output for the training example ***d*** and $\boldsymbol{o_d}$ is the output of the linear unit for training example ***d***.
- Given the above error definition, the error surface must be parabolic with a single global minimum.

Error Surface

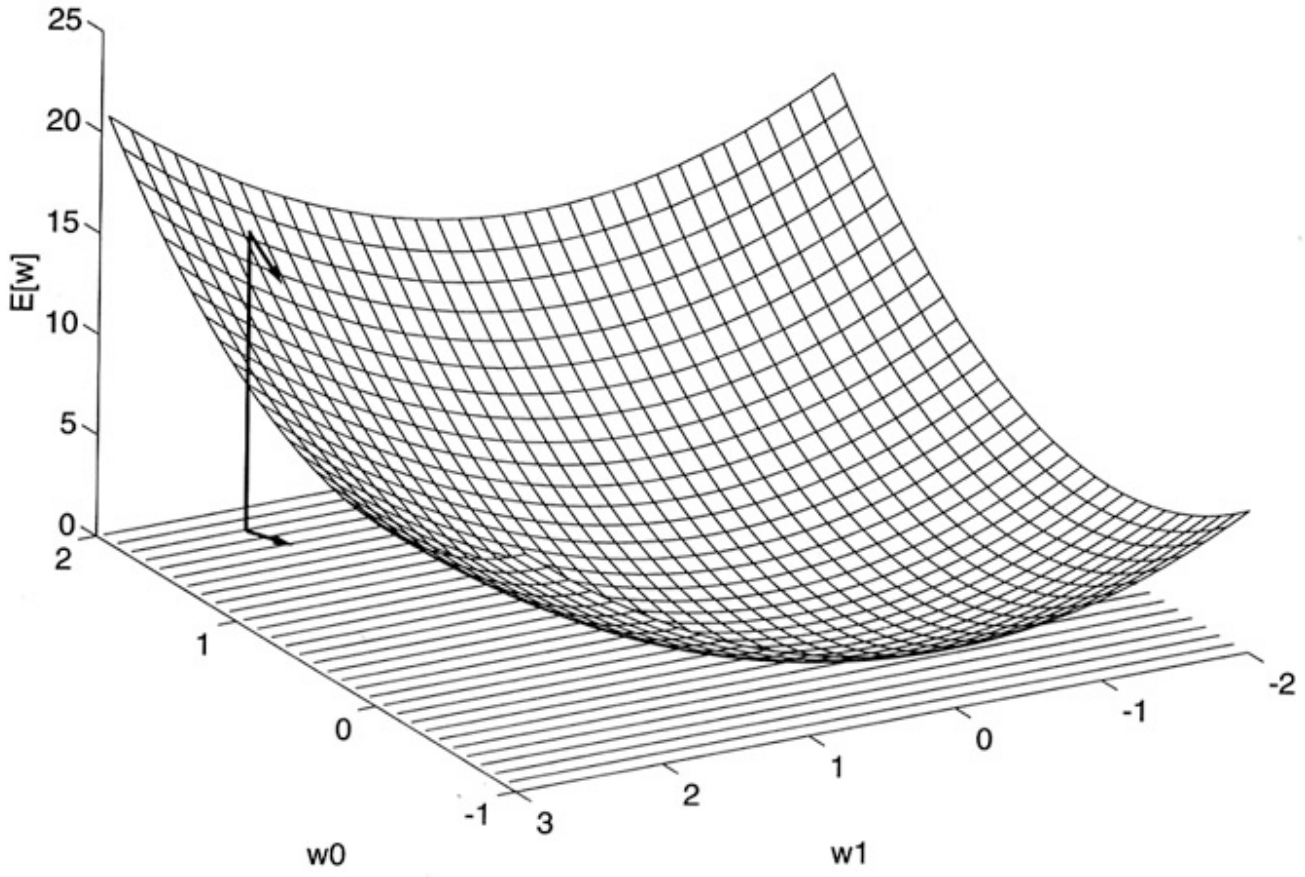


FIGURE 4.4

Gradient-Descent Algorithm

GRADIENT-DESCENT($training\_examples, \eta$)

Each training example is a pair of the form $\langle \vec{x}, t \rangle$, where $\vec{x}$ is the vector of input values, and t is the target output value. η is the learning rate (e.g., .05).

- Initialize each w_i to some small random value
- Until the termination condition is met, Do
  - Initialize each Δw_i to zero.
  - For each $\langle \vec{x}, t \rangle$ in $training\_examples$, Do
    - Input the instance $\vec{x}$ to the unit and compute the output o
    - For each linear unit weight w_i, Do

$$\Delta w_i \leftarrow \Delta w_i + \eta(t - o)x_i \tag{T4.1}$$

  - For each linear unit weight w_i, Do

$$w_i \leftarrow w_i + \Delta w_i \tag{T4.2}$$

Weight Update Rule

- Gradient descent determines the weight vector that minimizes E. It starts with an arbitrary weight vector, modifies it in small steps in the direction that produces the steepest descent, and continues until the global minimum error is reached,
- Weight update rule: $\Delta w_i = \eta \sum_{d \in D} (t_d - o_d) x_{id}$
- Where $\boldsymbol{x_{id}}$ denotes input component $\boldsymbol{x_i}$ for training example $\boldsymbol{d}$

Convergence

- Because the error surface contains only a single global minimum, the algorithm will converge to a weight vector with minimum error, regardless of whether the training examples are linearly separable, given a sufficiently small learning rate η is used.
- Hence a common modification is to gradually reduce the value of η as the number of steps grows.

Problems with Gradient descent

- Important general paradigm when
  1. Continuously parameterized hypothesis
  2. The error can be differentiated with respect to the hypothesis parameters
- The key practical problems are
  1. Converging to a local minimum can be quite slow
  2. If there are multiple local minima, then there is no guarantee that the procedure will find the global minimum (The error surface before will not be parabolic with a single global minima when training multiple nodes.)

Stochastic Gradient Descent

- Approximate gradient descent search by updating weights incrementally, following the calculation of the error for ***each*** individual example
- Delta rule: $\Delta w_i = \eta(t - o)x_i$
- (same as LMS algorithm, but only similar to perceptron training rule)
- Error function: $E_d(\vec{w}) = \frac{1}{2}(t_d - o_d)^2$
- If η is sufficiently small, stochastic gradient descent (SGD) can be made to approximate true gradient descent (GD) arbitrarily closely

Difference between GD and SGD

- In GD the error is summed over all examples before updating weights, in SGD weights are updated upon examining each training example
- Summing over multiple examples in GD requires more computation per weight update step. But since it uses the True gradient, it is often used with a larger step size (larger η).
- If there are multiple local minima with respect to E($\boldsymbol{w}$), SGD can sometimes avoid falling into these local minima. $\boldsymbol{w}$ is a vector variable

Delta Rule vs. Perceptron Training Rule

- Appear identical, but PTR is for thresholded perceptron and DR is for a linear unit (or unthresholded perceptron)
- DR can be used to train a thresholded perceptron, by using ±1 as target values to a linear unit, $o = \boldsymbol{w} \cdot \boldsymbol{x}$, and having the thresholded unit, $o' = \text{sgn}(\boldsymbol{w} \cdot \boldsymbol{x})$, where $\boldsymbol{w}$ and $\boldsymbol{x}$ are vector variables

Perceptron vs Linear Unit

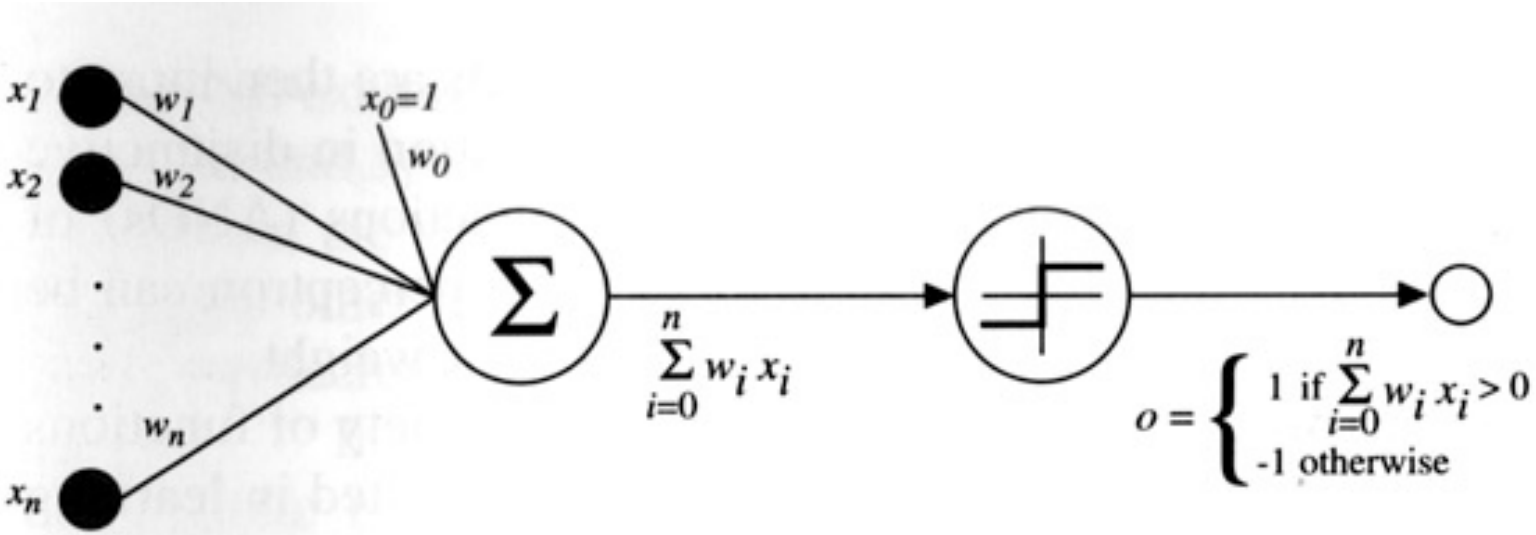
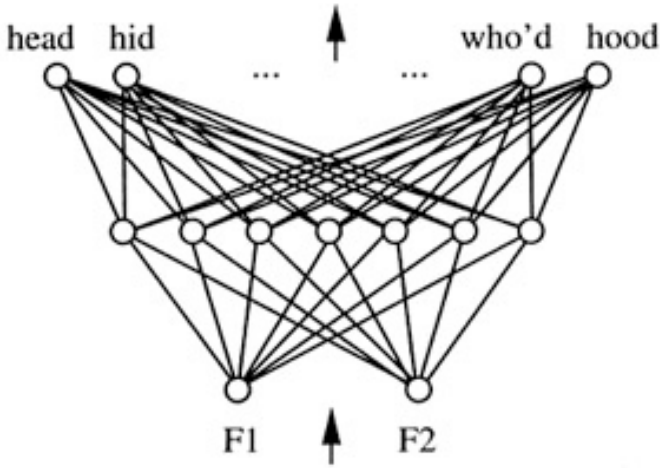


FIGURE 4.2
A perceptron.

Delta Rule with Unthresholded perceptron

- If the unthresholded perceptron can be trained to fit these values perfectly then so can the thresholded perceptron.
- If the target values cannot be perfectly fit, then the thresholded perceptron will be correct whenever the linear unit has the right sign, but this is not guaranteed to happen

Multilayer Networks & Nonlinear Surfaces



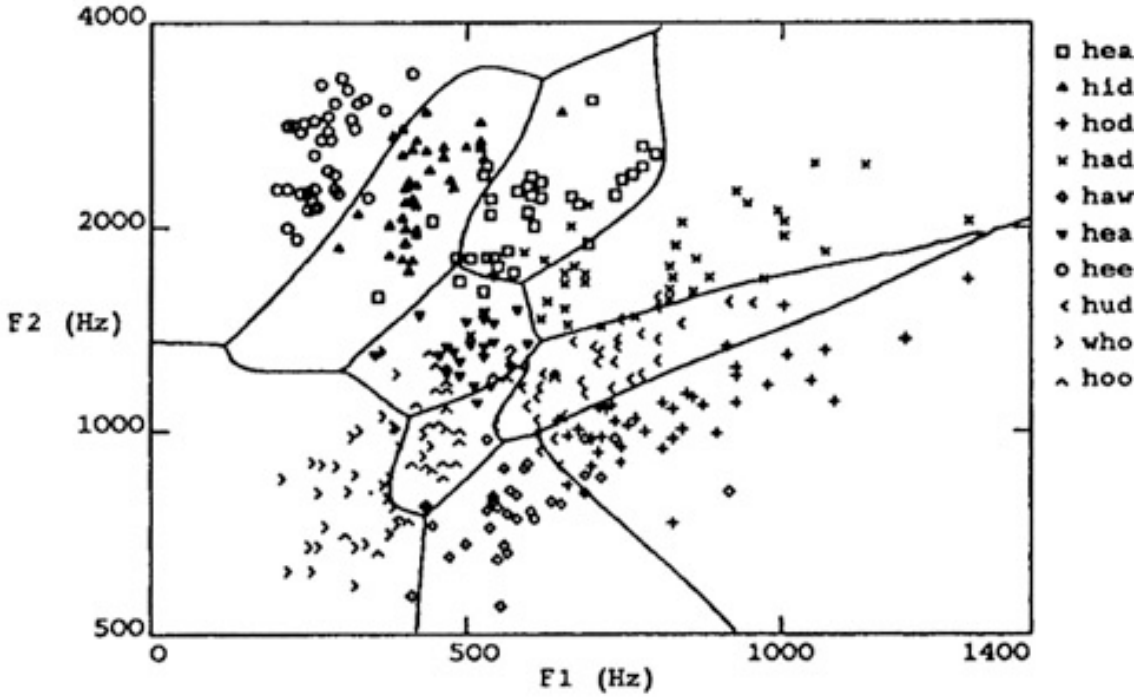


FIGURE 4.5

Multi layer Networks

- Multiple layers of linear units still produce only linear functions
- Perceptrons have a discontinuous threshold which is undifferentiable and therefore unsuitable for gradient descent
- We want a unit whose output is a nonlinear differentiable function of the inputs
- One solution is a sigmoid unit

What is a Sigmoid Unit?

- Like perceptrons it computes a linear combination of its inputs and then applies a threshold to the result. But the threshold output is a continuous function of its input which ranges from 0 to 1.
- If is often referred to as a squashing function.

Sigmoid Threshold Unit

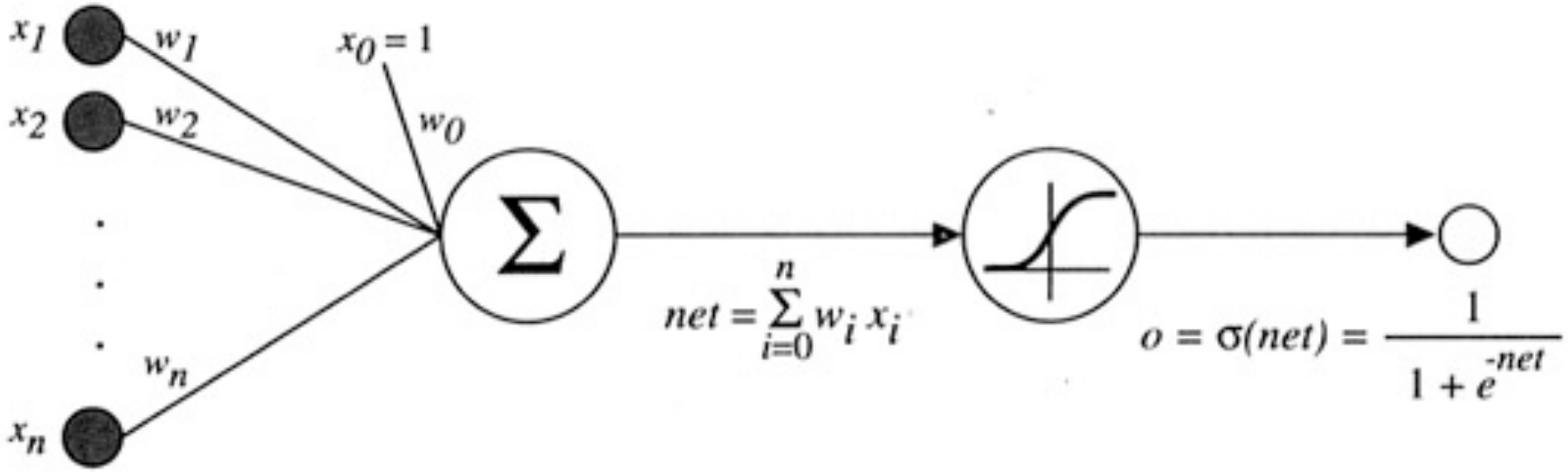


FIGURE 4.6

Properties of the Backpropagation Algorithm

- Learns weights for a multilayer network, given a fixed set of units and interconnections
- It uses gradient descent to minimize the squashed error between the network outputs and the target values for these outputs

Error surface

- Error formula: $E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{kd} - o_{kd})^2$
- ***Outputs*** is the set of output units in the network, t_{kd} and o_{kd} are the target value and output value associated with the k^{th} output unit and the training example ***d***
- In multilayer networks the error surface can have multiple minima, but in practice Backpropagation has produced excellent results in many real-world applications
- The algorithm is for two layers of sigmoid units and does stochastic gradient descent

Backpropagation Algorithm

BACKPROPAGATION($training\_examples, \eta, n_{in}, n_{out}, n_{hidden}$)

Each training example is a pair of the form $\langle \vec{x}, \vec{t} \rangle$, *where* $\vec{x}$ *is the vector of network input values, and* $\vec{t}$ *is the vector of target network output values.*

η *is the learning rate (e.g., .05).* n_{in} *is the number of network inputs,* n_{hidden} *the number of units in the hidden layer, and* n_{out} *the number of output units.*

The input from unit i *into unit* j *is denoted* x_{ji}, *and the weight from unit* i *to unit* j *is denoted* w_{ji}.

- Create a feed-forward network with n_{in} inputs, n_{hidden} hidden units, and n_{out} output units.
- Initialize all network weights to small random numbers (e.g., between $-.05$ and .05).
- Until the termination condition is met, Do
  - For each $\langle \vec{x}, \vec{t} \rangle$ in $training\_examples$, Do

Propagate the input forward through the network:

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

Propagate the errors backward through the network:

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

$$\delta_k \leftarrow o_k(1 - o_k)(t_k - o_k) \tag{T4.3}$$

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

$$\delta_h \leftarrow o_h(1 - o_h) \sum_{k \in outputs} w_{kh}\delta_k \tag{T4.4}$$

4. Update each network weight w_{ji}

$$w_{ji} \leftarrow w_{ji} + \Delta w_{ji}$$

where

$$\Delta w_{ji} = \eta \, \delta_j \, x_{ji} \tag{T4.5}$$

Backpropogation Weight Training Rule

- The error ***(t-o)*** in the delta rule is replaced by δ_j
- For output unit ***k*** it is the familiar $(t_k - o_k)$ from the delta rule multiplied by $o_k(1-o_k)$ which is the derivative of the sigmoid squashing function
- For hidden unit ***h*** the derivative component is the same but there is no target value directly available so you sum the error terms δ_k for each output unit influenced by ***h*** weighing each of the δ_k by the weight, w_{kh}, from the hidden unit ***h*** to the output unit ***k***.
- This weight characterizes the degree to which each hidden unit ***h*** is responsible for the error in output unit ***k***.

Termination Conditions for Backpropagation

- Halt after a fixed number of iterations
- Once the error on the training examples falls below some threshold
- Once the error on a separate validation set of examples meets some criterion
- Important:
  - Too few iterations - fail to reduce error sufficiently
  - Too many iterations - overfit the data

Momentum

- Making the weight in the nth iteration depend partially on the update during the $(n\text{-}1)^{th}$ iteration

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

- The momentum is represented by $\boldsymbol{0 \leq \alpha < 1}$

Intuition behind Momentum

- The gradient search trajectory is analogous to a momentumless ball rolling down the error surface, the effect of α is to keep the ball rolling in the same direction from one iteration to the next
- The ball can roll through small local minima or along flat regions in the surface where the ball would stop without momentum
- It also causes a gradual increase in the step size in regions where the gradient is unchanging thereby speeding convergence

Arbitrary Acyclic Networks

- Only equation (T4.4) has to change
- Feedforward networks of arbitrary depth

$$\delta_r = o_r(1 - o_r) \sum_{s \in layer\, m+1} w_{sr}\delta_s$$

- Directed acyclic graph, not arranged in uniform layers

$$\delta_r = o_r(1 - o_r) \sum_{s \in Downstream(r)} w_{sr}\delta_s$$

Convergence and Local Minima

- The error surface in multilayer neural networks may contain many different local minima where gradient descent can become trapped
- But backpropagation is a highly effective function approximation in practice
- Why??

Why it works

- Networks with large numbers of weights correspond to error surfaces in very high dimensional spaces
- When gradient descent falls into a local minima with respect to one weight it won't necessarily be with respect to the other weights
- The more weights, the more dimensions that might provide an escape route
  - do I believe this??? - more nodes, more outputs, more inputs

Heuristics to Overcome Local Minima

- Add momentum
- Use stochastic gradient search
- New seed (e.g., initial random weights), and choose the one with the best performance on the validation set or treat as a committee or ensemble

Representational Power of Feedforward Networks

- Boolean functions: 2 layers of units, but number of hidden nodes grows exponentially in the number of inputs
- Continuous Functions: every bounded continuous function to **arbitrary accuracy** in two layers of units
- Arbitrary functions: **arbitrary accuracy** by a network with 3 layers of units - based on linear combination of many localized functions

Caveats

- Arbitrary error???

- Network weight variables reachable from the initial weight values may not include all possible weight vectors

Hypothesis Space

- Every possible assignment of network weights represents a syntactically different hypothesis
- N-dimensional Euclidean space of the n network weights
- This hypothesis space is continuous
- Since E is differentiable with respect to the continuous parameters, we have a well-defined error gradient

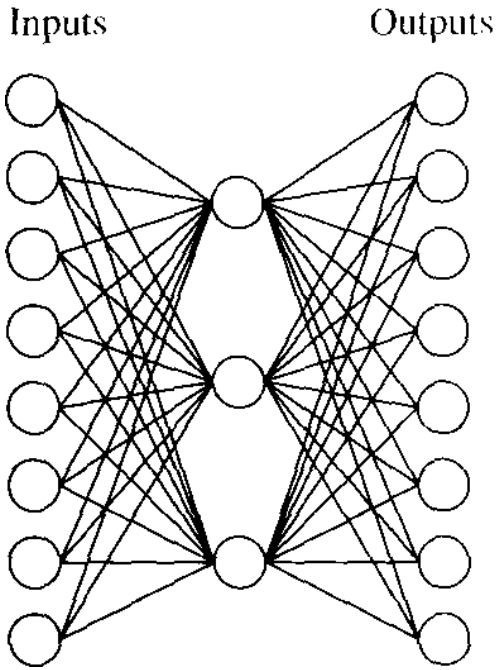
Inductive Bias

- Inductive Bias depends on interplay between gradient descent search and the way the weight space spans the space of representable functions
- Roughly - smooth interpolation between data points
- Given two positive training instances with no negatives between them. Backpropagation will tend to label the points between as positive.

Hidden Layer Representations

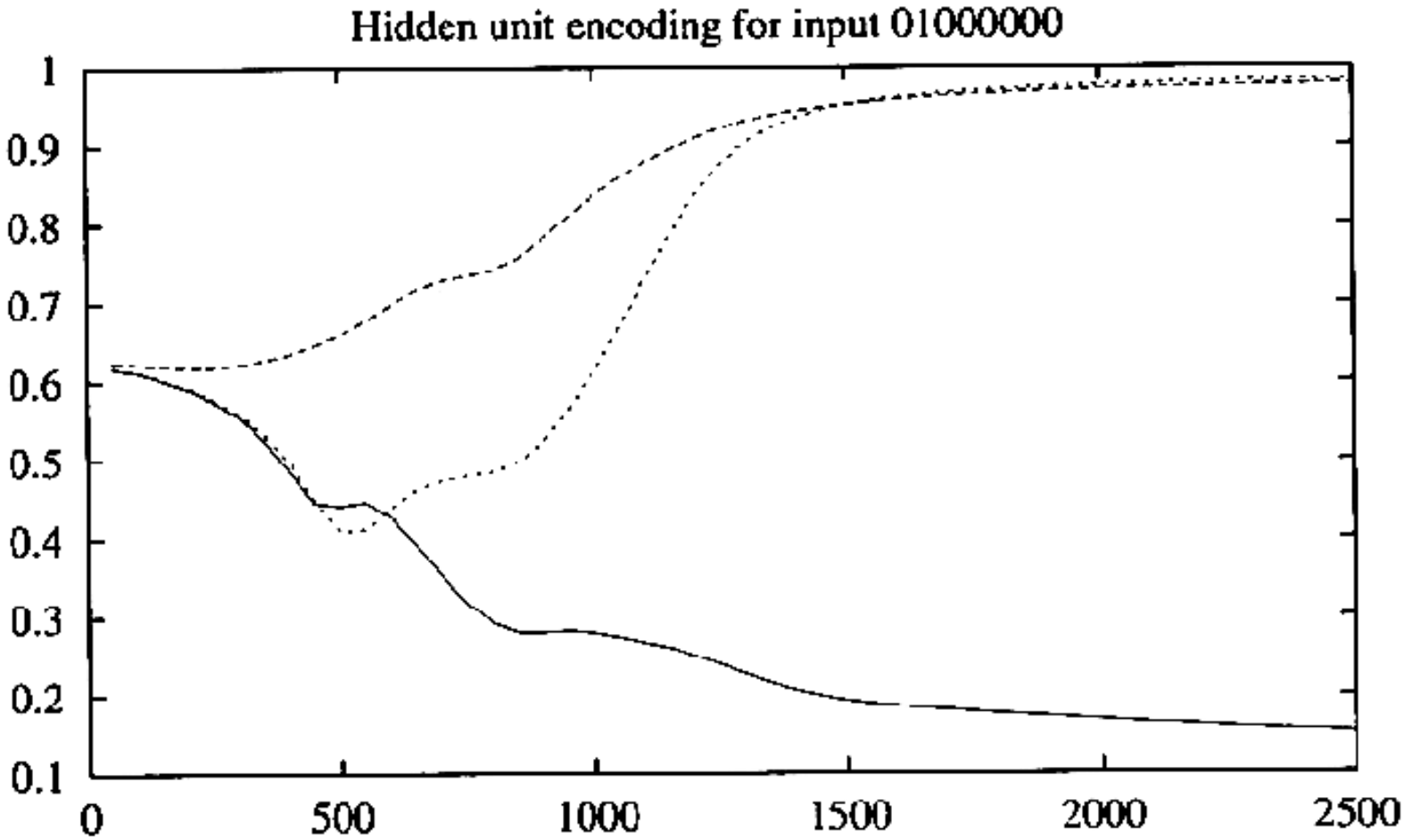
- Backpropagation can discover useful intermediate representations at the hidden unit layers
- It is a way to make implicit concepts explicit (not across rows!)
- Discovering binary encoding
- Important degree of flexibility
- More layers of units - more complex features can be invented

Backprop in action

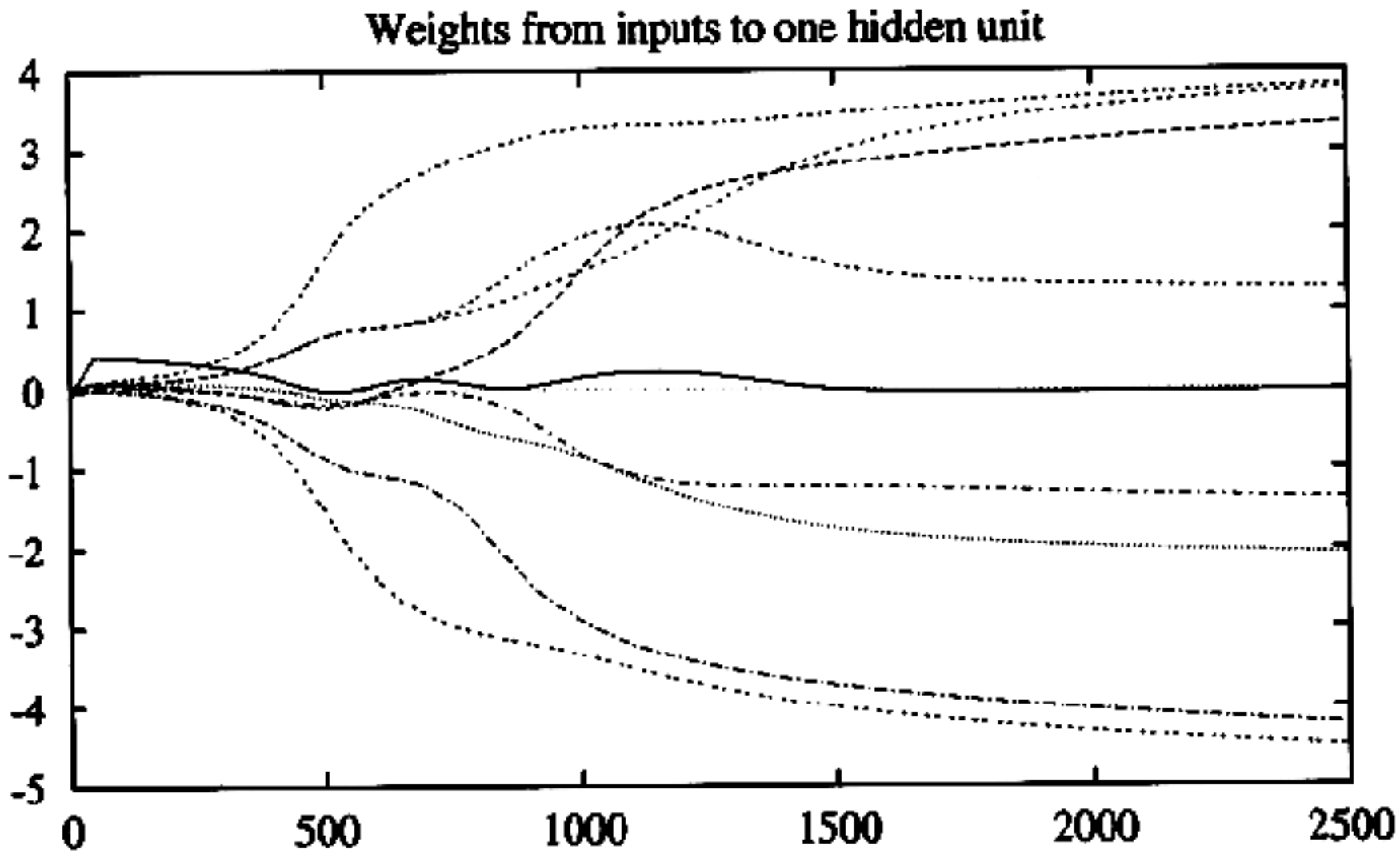


Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.15	.99	.99	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.01	.11	.88	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

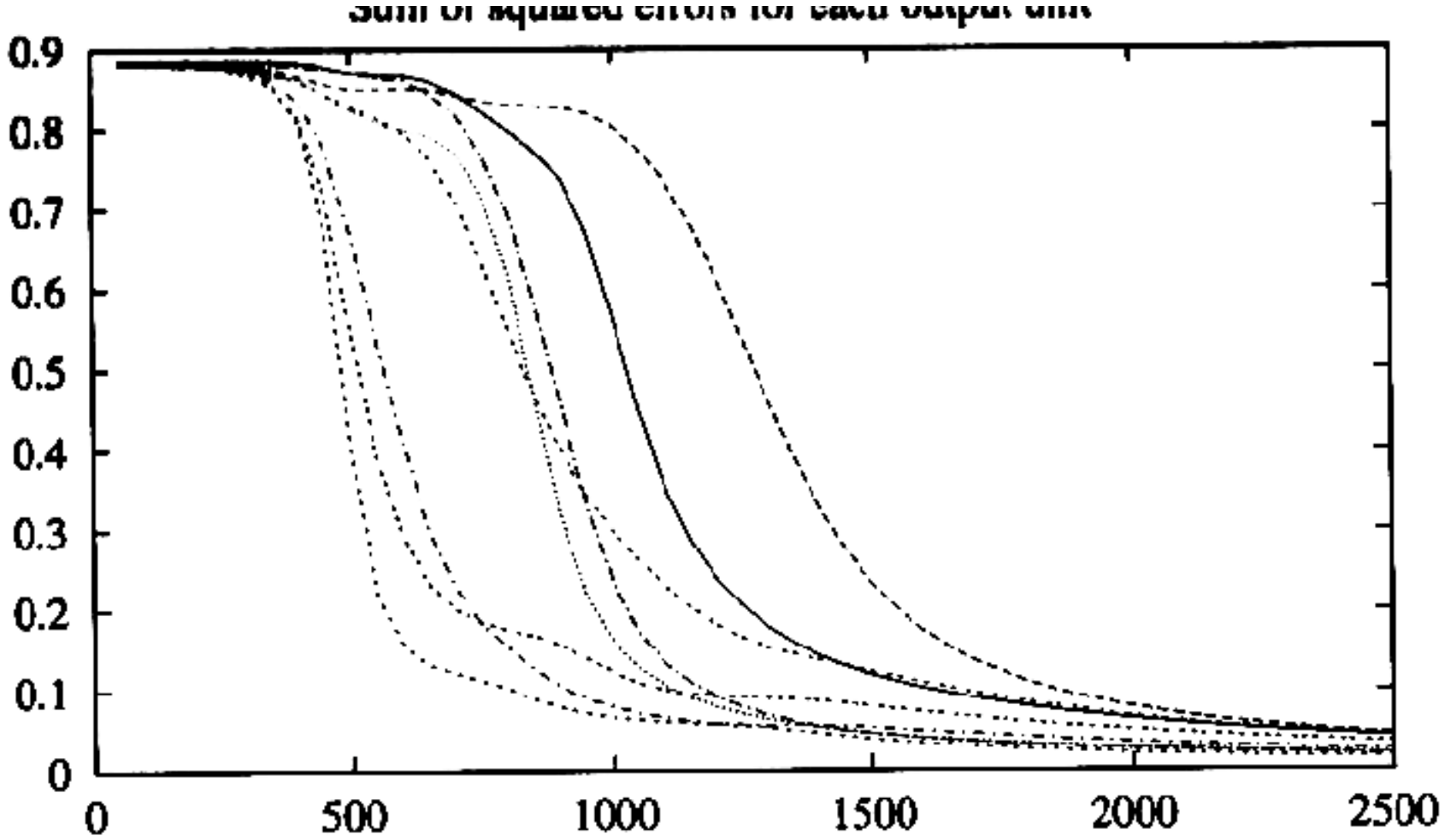
Hidden Unit Encoding



Weights from inputs



Sum of squares Error



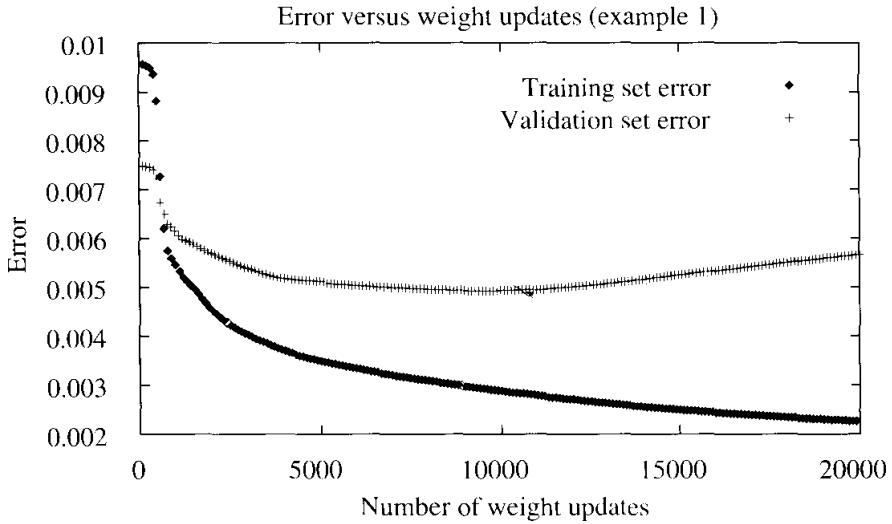
Overfitting and Stopping Criteria

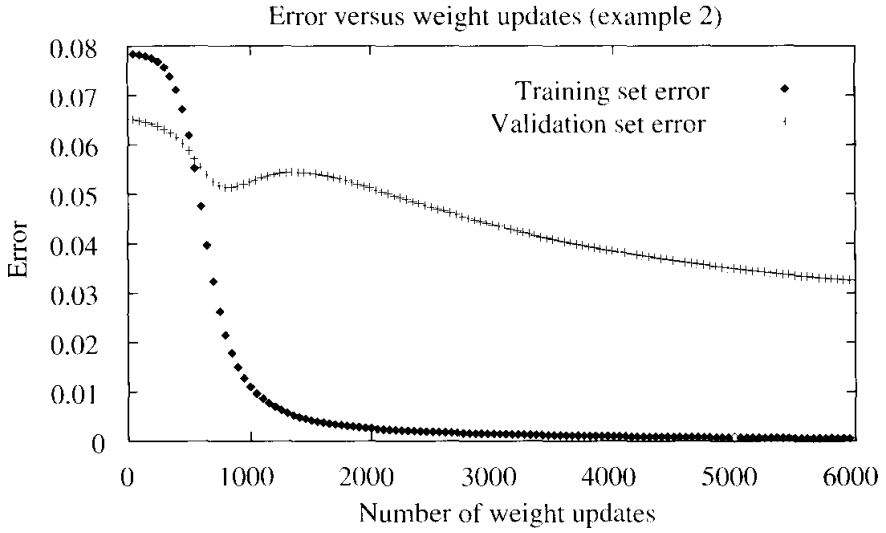
1. Train until the E on the training examples falls below some level
   - Why does overfitting tend to occur in later iterations?
   - Initially weights are set to small random numbers, as training proceeds weights change to reduce error over the training data & complexity of the decision surface increases, given enough iterations can overfit. Again error space vs function space???
   - Weight decay - decreases each weight by a small factor on each iteration - intuition keep weight values small to bias against complex decision surfaces - do complex decision surfaces need to have high weights???

Continued

2. Stop when you reach the lowest error on the validation set
   - Keep current ANN weights and the best-performing weights thus far measured by error over the validation set
   - Training is terminated once the current weights reach a significantly higher error over the validation set
   - Care must be taken to avoid stopping too soon!!
   - If data is too small can do k-fold cross validation (remember to use just to determine the number of iterations!) then train over whole dataset (same in decision trees)

Error Plots


Error versus weight updates (example 1)
Training set error
Validation set error
Error
0.01
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0
5000
10000
15000
20000
Number of weight updates


Error versus weight updates (example 2)
Training set error
Validation set error
Error
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
1000
2000
3000
4000
5000
6000
Number of weight updates

Face Recognition Task

- 20 people
- 32 images per person
- Varying expression, direction looking, wearing sunglasses, background, clothing worn, position of face in image
- 624 greyscale images, resolution 120x128, each pixel intensity ranges from 0 to 255
- Could be many targets: identity, direction, gender, whether wearing sunglasses - All can be learned to high accuracy
- We consider direction looking

Input Encoding

- How encode the image?

- Use 102x128 inputs?
- Extract local features: edges, regions of uniform intensity - how handle a varying number of features per image?

Actual Input Encoding Used

- Encode image in 30x32 pixel intensity values, with one network input per pixel - pixel intensities were linearly scaled from 0 to 255 down to 0 to 1. Why?
- The 30x32 grid is a coarse resolution summary. Coarse pixel intensity is a mean of the corresponding high pixel intensities - reduces computational demands while maintaining sufficient resolution to correctly classify images - same as ALVINN except there a represented pixel was chosen randomly for efficiency

Output Encoding

- A single output unit, assigning 0.2, 0.4, 0.6, 0.8 as being left, right, up and straight

  OR

- Have 4 output nodes and choose the highest-valued output as the prediction (1-of-n output encoding)

Output Encoding Issues

- Is “left” really closer to “right” then it is to “up”?
- 4 outputs gives more degrees of freedom to the network for representing the target function (4x #hidden units instead of 1x)
- The difference between the highest valued output and the second highest valued output gives a measure of the confidence in the network prediction

Target Values

- What should the target values be?

- Could use <1,0,0,0> but we use <0.9,0.1,0.1,0.1> - sigmoid units can't produce 0 and 1 exactly with finite weights so gradient descent will force the weights to grow without bound

Network Graph Structure

- How many units and how to interconnect?
- Most common - layer units with feedforward connections from every unit in one layer to every unit in the next
- The more layers the longer the training time - we choose 1 hidden layer and 1 output layer

Hidden Units

- How many hidden units?
  - 3 units = 90% accuracy, 5 minutes learning time
  - 30 units = 92% accuracy, 1 hr learning time
- In general there is a minimum number of hidden units needed and above that the extra hidden units do not dramatically effect the accuracy, provided cross-validation is used to determine how many gradient descent iterations should be performed, otherwise increasing the number of hidden units often increases the tendency to overfit the training data

Other Algorithm Parameters

- Learning rate, η, was set to 0.3
- Momentum, α, was set to 0.3
- Lower values produced equivalent generalization but longer training times, if set too high training fails to converge to a network with acceptable error
- Full gradient descent was used (not the stochastic approximation)

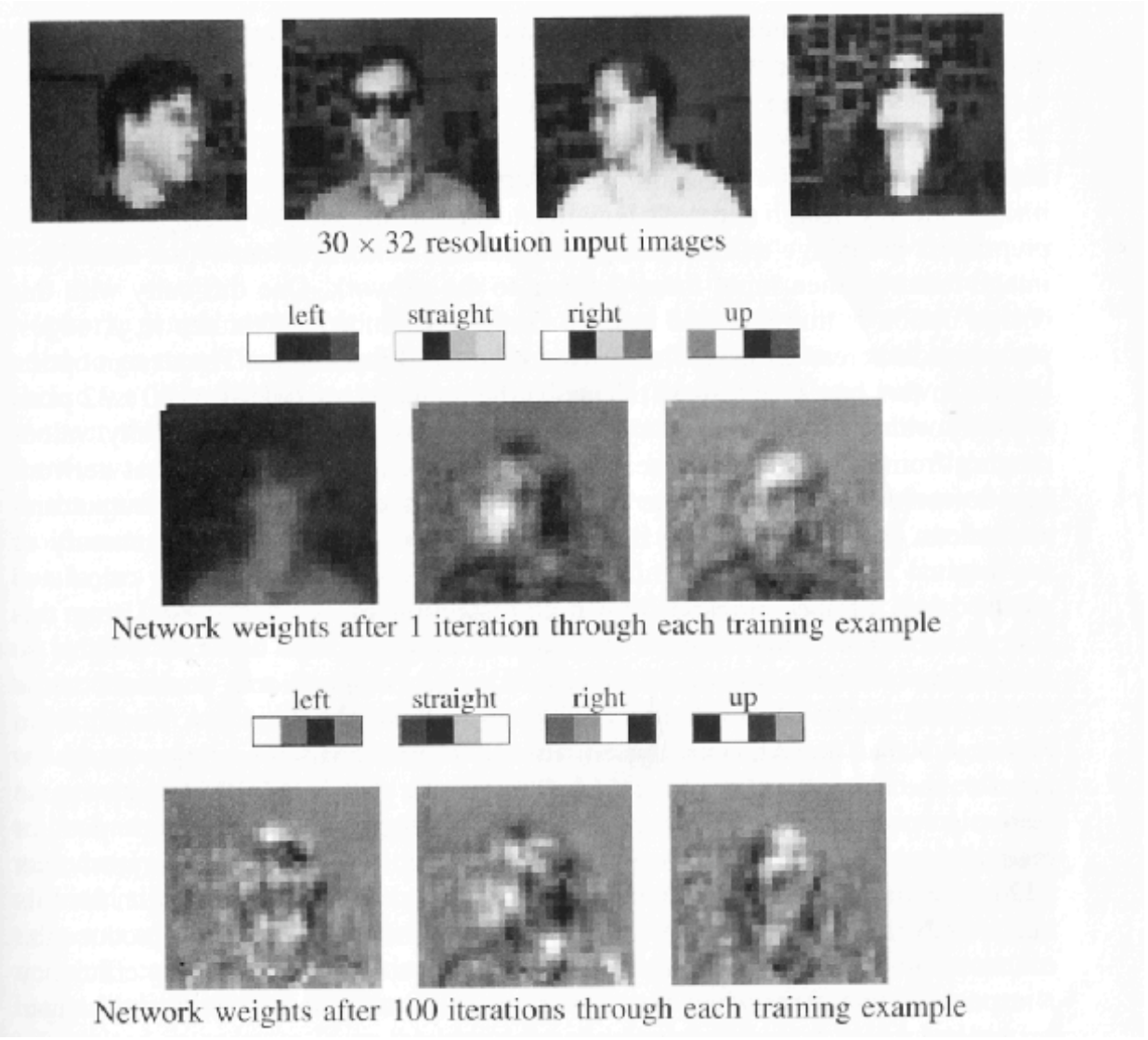
More Parameters

- Network weights in the output units were initialized to small random values, but the input unit weights were initialized to zero because it yields a more intelligible visualization of the learned weights without noticeable impact on generalization accuracy

Still More Parameters

- The number of training iterations was selected by partitioning the available data into a training set and a separate validation set, GD was used to minimize the error over the training set and after every 50 gradient descent steps the network performance was evaluated over the validation set. The final reported accuracy was measured over yet a third set of test examples that were not use to influence the training.

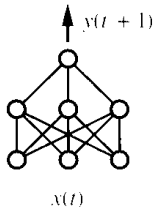
Learned Hidden Representations



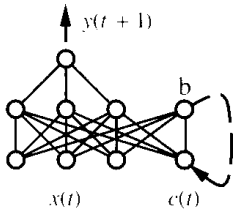
Advanced Topics

- Alternative Error Functions
- Alternative Error Minimization Procedures
- Recurrent Networks
- Dynamically Modifying Network Structure

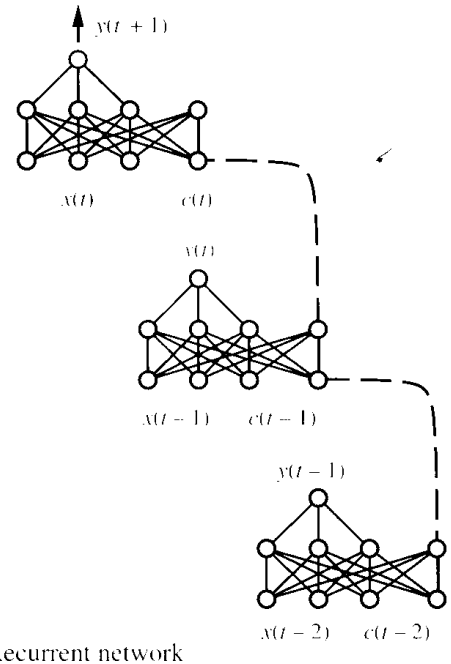
Recurrent Neural Networks



(a) Feedforward network



(b) Recurrent network



(c) Recurrent network unfolded in time

Summary

- Practical method for learning real-valued and vector-valued functions over continuous and discrete-valued attributes
- Robust to noise in the training data
- Backpropagation algorithm is the most common
- Hypothesis space: all functions that can be represented by assigning weights to the fixed network of interconnected units
- Feedforward networks containing 3 layers can approximate any function to arbitrary accuracy given sufficient number of units in each layer

Summary II

- Networks of practical size are capable of representing a rich space of highly nonlinear functions
- Backpropagation searches the space of possible hypotheses using gradient descent (GD) to iteratively reduce the error in the network to fit the training data.
- GD converges to a local minimum in the training error with respect to the network weights
- Backpropagation has the ability to invent new features that are not explicit in the input

Summary III

- Hidden units of multilayer networks learn to represent intermediate features (e.g., face recognition)
- Overfitting is an important issue (caused by overuse of accuracy IMHO)
- Cross-validation can be used to estimate an appropriate stopping point for gradient descent
- Many other algorithms and extensions.