Artificial Neural Networks

[Read Ch. 4]
[Recommended exercises 4.1, 4.2, 4.5, 4.9, 4.11]

- Threshold units
- Gradient descent
- Multilayer networks
- Backpropagation
- Hidden layer representations
- Example: Face Recognition
- Advanced topics
Connectionist Models

Consider humans:

- Neuron switching time \( \sim .001 \) second
- Number of neurons \( \sim 10^{10} \)
- Connections per neuron \( \sim 10^{4-5} \)
- Scene recognition time \( \sim .1 \) second
- 100 inference steps doesn’t seem like enough
  \[\rightarrow\] much parallel computation

Properties of artificial neural nets (ANN’s):

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed process
- Emphasis on tuning weights automatically
When to Consider Neural Networks

- Input is high-dimensional discrete or real-valued (e.g. raw sensor input)
- Output is discrete or real valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant

Examples:

- Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial prediction
Perceptron

\[ o(x_1, \ldots, x_n) = \begin{cases} 
1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\
-1 & \text{otherwise.} 
\end{cases} \]

Sometimes we’ll use simpler vector notation:

\[ o(\vec{x}) = \begin{cases} 
1 & \text{if } \vec{w} \cdot \vec{x} > 0 \\
-1 & \text{otherwise.} 
\end{cases} \]
Decision Surface of a Perceptron

Represents some useful functions

- What weights represent
  \[ g(x_1, x_2) = AND(x_1, x_2) \]?

But some functions not representable

- e.g., not linearly separable
- Therefore, we’ll want networks of these...
Perceptron training rule

\[ w_i \leftarrow w_i + \Delta w_i \]

where

\[ \Delta w_i = \eta(t - o)x_i \]

Where:

- \( t = c(\vec{x}) \) is target value
- \( o \) is perceptron output
- \( \eta \) is small constant (e.g., .1) called learning rate
Perceptron training rule

Can prove it will converge

- If training data is linearly separable
- and $\eta$ sufficiently small
Gradient Descent

To understand, consider simpler linear unit, where

$$o = w_0 + w_1 x_1 + \cdots + w_n x_n$$

Let’s learn $w_i$’s that minimize the squared error

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

Where $D$ is set of training examples
Gradient Descent

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

Training rule:

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

i.e.,

\[ \Delta w_i = -\eta \frac{\partial E}{\partial w_i} \]
Gradient Descent

\[
\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 = \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 = \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) = \sum_d (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{w} \cdot \vec{x}_d)
\]

\[
\frac{\partial E}{\partial w_i} = \sum_d (t_d - o_d) (-x_{i,d})
\]
Gradient Descent

\textsc{Gradient-Descent}(training\_examples, \eta)

Each training example is a pair of the form \langle \bar{x}, t \rangle, where \bar{x} is the vector of input values, and \( t \) is the target output value. \( \eta \) 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 \( \Delta w_i \) to zero.
  - For each \( \langle \bar{x}, t \rangle \) in training\_examples, Do
    * Input the instance \( \bar{x} \) to the unit and compute the output \( o \)
    * For each linear unit weight \( w_i \), Do
      \[ \Delta w_i \leftarrow \Delta w_i + \eta(t - o)x_i \]
  - For each linear unit weight \( w_i \), Do
    \[ w_i \leftarrow w_i + \Delta w_i \]
Summary

Perceptron training rule guaranteed to succeed if
- Training examples are linearly separable
- Sufficiently small learning rate $\eta$

Linear unit training rule uses gradient descent
- Guaranteed to converge to hypothesis with minimum squared error
- Given sufficiently small learning rate $\eta$
- Even when training data contains noise
- Even when training data not separable by $H$
Incremental (Stochastic) Gradient Descent

**Batch mode** Gradient Descent:
Do until satisfied
1. Compute the gradient $\nabla E_D[\vec{w}]$
2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_D[\vec{w}]$

**Incremental mode** Gradient Descent:
Do until satisfied
- For each training example $d$ in $D$
  1. Compute the gradient $\nabla E_d[\vec{w}]$
  2. $\vec{w} \leftarrow \vec{w} - \eta \nabla E_d[\vec{w}]$

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

*Incremental Gradient Descent* can approximate *Batch Gradient Descent* arbitrarily closely if $\eta$ made small enough
Multilayer Networks of Sigmoid Units
Sigmoid Unit

[Diagram]

\[ \sigma(x) \text{ is the sigmoid function} \]

\[ \sigma(x) = \frac{1}{1 + e^{-x}} \]

Nice property: \[ \frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x)) \]

We can derive gradient decent rules to train

- One sigmoid unit
- Multilayer networks of sigmoid units → Backpropagation
Error Gradient for a Sigmoid Unit

\[
\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2
\]

\[
= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2
\]

\[
= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d)
\]

\[
= \sum_d (t_d - o_d) \left( - \frac{\partial o_d}{\partial w_i} \right)
\]

\[
= - \sum_d (t_d - o_d) \frac{\partial o_d}{\partial \text{net}_d} \frac{\partial \text{net}_d}{\partial w_i}
\]

But we know:

\[
\frac{\partial o_d}{\partial \text{net}_d} = \frac{\partial \sigma(\text{net}_d)}{\partial \text{net}_d} = o_d(1 - o_d)
\]

\[
\frac{\partial \text{net}_d}{\partial w_i} = \frac{\partial (\vec{w} \cdot \vec{x}_d)}{\partial w_i} = x_{i,d}
\]

So:

\[
\frac{\partial E}{\partial w_i} = - \sum_{d \in D} (t_d - o_d) o_d(1 - o_d) x_{i,d}
\]
Backpropagation Algorithm

Initialize all weights to small random numbers. Until satisfied, Do

• For each training example, Do

  1. Input the training example to the network and compute the network outputs

  2. For each output unit \( k \)

     \[
     \delta_k \leftarrow o_k(1 - o_k)(t_k - o_k)
     \]

  3. For each hidden unit \( h \)

     \[
     \delta_h \leftarrow o_h(1 - o_h) \sum_{k \in \text{outputs}} w_{h,k} \delta_k
     \]

  4. Update each network weight \( w_{i,j} \)

     \[
     w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}
     \]

     where

     \[
     \Delta w_{i,j} = \eta \delta_j x_{i,j}
     \]
More on Backpropagation

- Gradient descent over entire network weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight momentum $\alpha$
  \[ \Delta w_{i,j}(n) = \eta \delta_j x_{i,j} + \alpha \Delta w_{i,j}(n-1) \]
- Minimizes error over training examples
  - Will it generalize well to subsequent examples?
- Training can take thousands of iterations → slow!
- Using network after training is very fast
Learning Hidden Layer Representations

A target function:

<table>
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<tr>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
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<tr>
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<td>00000001</td>
</tr>
</tbody>
</table>

Can this be learned??
Learning Hidden Layer Representations

A network:

Learned hidden layer representation:

<table>
<thead>
<tr>
<th>Input</th>
<th>Hidden Values</th>
<th>Output</th>
</tr>
</thead>
<tbody>
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<tr>
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<td>00000001</td>
</tr>
</tbody>
</table>
Training

Sum of squared errors for each output unit
Training
Training

Weights from inputs to one hidden unit
Convergence of Backpropagation

Gradient descent to some local minimum

- Perhaps not global minimum...
- Add momentum
- Stochastic gradient descent
- Train multiple nets with different initial weights

Nature of convergence

- Initialize weights near zero
- Therefore, initial networks near-linear
- Increasingly non-linear functions possible as training progresses
Expressive Capabilities of ANNs

Boolean functions:

- Every boolean function can be represented by network with single hidden layer
- but might require exponential (in number of inputs) hidden units

Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].
Overfitting in ANNs

Error versus weight updates (example 1)

Error versus weight updates (example 2)
Neural Nets for Face Recognition

90% accurate learning head pose, and recognizing 1-of-20 faces
Learned Hidden Unit Weights

![Diagram of a network with inputs labeled left, str, right, up, and learned weights for 30x32 inputs.]

Typical input images

http://www.cs.cmu.edu/~tom/faces.html
Alternative Error Functions

Penalize large weights:

\[
E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in \text{outputs}} (t_{kd} - o_{kd})^2 + \gamma \sum_{i,j} w_{ji}^2
\]

Train on target slopes as well as values:

\[
E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in \text{outputs}} \left[ (t_{kd} - o_{kd})^2 + \mu \sum_{j \in \text{inputs}} \left( \frac{\partial t_{kd}}{\partial x_d^j} - \frac{\partial o_{kd}}{\partial x_d^j} \right)^2 \right]
\]

Tie together weights:

- e.g., in phoneme recognition network
Recurrent Networks

(a) Feedforward network

(b) Recurrent network

(c) Recurrent network unfolded in time
Cognitive Neuroscience Models Based on ANN’s

Figure 4 | The process of differentiation of conceptual representations. The representations are those seen in the feedforward network model shown in Fig. 3. a | Acquired patterns of activation that represent the eight objects in the training set at three points in the learning process (epochs 250, 750 and 2,500). Early in learning, the patterns are undifferentiated; the first difference to appear is between plants and animals. Later, the patterns show clear differentiation at both the superordinate (plant–animal) and intermediate (bird–fish/tree–flower) levels. Finally, the individual concepts are differentiated, but the overall hierarchical organization of the similarity structure remains. b | A standard hierarchical clustering analysis program has been used to visualize the similarity structure in the