Classification / Regression

Neural Networks 2
Neural networks

- Topics
  - Perceptrons
    - structure
    - training
    - expressiveness
  - Multilayer networks
    - possible structures
      - activation functions
    - training with gradient descent and backpropagation
    - expressiveness
Neural network application

ALVINN: An Autonomous Land Vehicle In a Neural Network
(Carnegie Mellon University Robotics Institute, 1989-1997)

ALVINN is a perception system which learns to control the NAVLAB vehicles by watching a person drive. ALVINN's architecture consists of a single hidden layer back-propagation network. The input layer of the network is a 30x32 unit two dimensional "retina" which receives input from the vehicles video camera. Each input unit is fully connected to a layer of five hidden units which are in turn fully connected to a layer of 30 output units. The output layer is a linear representation of the direction the vehicle should travel in order to keep the vehicle on the road.
Neural network application

ALVINN drives 70 mph on highways!
General structure of multilayer neural network

Training multilayer neural network means learning the weights of inter-layer connections.
Neural network architectures

- All multilayer neural network architectures have:
  - At least one hidden layer
  - Feedforward connections from inputs to hidden layer(s) to outputs

but more general architectures also allow for:
- Multiple hidden layers
- Recurrent connections
  - from a node to itself
  - between nodes in the same layer
  - between nodes in one layer and nodes in another layer above it
Neural network architectures

More than one hidden layer

Recycled variables

Input variables

Bias

B1

B2

H1

H2

H3

H4

O1

O2

Output variables

Recurrent connections

Input Pattern (Vector)
Neural networks: roles of nodes

- A node in the input layer:
  - distributes value of some component of input vector to the nodes in the first hidden layer, without modification

- A node in a hidden layer(s):
  - forms weighted sum of its inputs
  - transforms this sum according to some activation function (also known as transfer function)
  - distributes the transformed sum to the nodes in the next layer

- A node in the output layer:
  - forms weighted sum of its inputs
  - (optionally) transforms this sum according to some activation function
Neural network activation functions

- Linear function
- Sigmoid function
- Tanh function
- Sign function
The architecture most widely used in practice is fairly simple:

- One hidden layer
- No recurrent connections (feedforward only)
- Non-linear activation function in hidden layer (usually sigmoid or tanh)
- No activation function in output layer (summation only)

This architecture can model any bounded continuous function.
Neural network architectures

Regression

Input Layer

Hidden Layer

Output Layer

continuous y

Classification: two classes

Input Layer

Hidden Layer

Output Layer

continuous plus threshold → 0/1 classes
Neural network architectures

Classification: multiple classes

Input Layer

Hidden Layer

Output Layer

continuous plus max $\rightarrow 1$ of $k$ classes
Classification: multiple classes

- When outcomes are one of \( k \) possible classes, they can be encoded using \( k \) dummy variables.
  - If an outcome is class \( j \), then \( j \)th dummy variable = 1, all other dummy variables = 0.

- Example with four class labels:

\[
y_i = \begin{pmatrix}
1 \\
3 \\
2 \\
2 \\
4 \\
1
\end{pmatrix} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0
\end{pmatrix}
\]
**Algorithm for learning neural network**

- Initialize the connection weights \( \mathbf{w} = (w_0, w_1, \ldots, w_m) \)
  - \( \mathbf{w} \) includes all connections between all layers
  - Usually small random values
- Adjust weights such that output of neural network is consistent with class label / dependent variable of training samples
  - Typical loss function is squared error:
    \[
    E(\mathbf{w}) = \sum_i [y_i - \hat{y}_i]^2 = \sum_i [y_i - f(\mathbf{w}, \mathbf{x}_i)]^2
    \]
  - Find weights \( w_j \) that minimize above loss function
Sigmoid unit

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

\[ \frac{1}{1 + e^{-x}} \]

Nice property: \( \frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x)) \)
Sigmoid unit: training

- We can derive gradient descent rules to train:
  - A single sigmoid unit
  - Multilayer networks of sigmoid units
    - referred to as backpropagation
Backpropagation

Example: stochastic gradient descent, feedforward network with two layers of sigmoid units

Do until convergence

For each training sample \( i = \langle x_i, y_i \rangle \)

Propagate the input forward through the network

Calculate the output \( o_h \) of every hidden unit

Calculate the output \( o_k \) of every network output unit

Propagate the errors backward through the network

For each network output unit \( k \), calculate its error term \( \delta_k \)

\[
\delta_k = o_k (1 - o_k) (y_{ik} - o_k)
\]

For each hidden unit \( h \), calculate its error term \( \delta_h \)

\[
\delta_h = o_h (1 - o_h) \sum_k (w_{hk} \delta_k)
\]

Update each network weight \( w_{ba} \)

\[
w_{ba} = w_{ba} + \eta \delta_b z_{ba}
\]

where \( z_{ba} \) is the \( a \)th input to unit \( b \)
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 $\rightarrow$ slow!
- Using network after training is very fast
MATLAB interlude

matlab_demo_14.m

neural network classification of crab gender

200 samples
6 features
2 classes
Neural networks for data compression
Neural networks for data compression

A target function:

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>10000000</td>
<td>→ 10000000</td>
</tr>
<tr>
<td>01000000</td>
<td>→ 01000000</td>
</tr>
<tr>
<td>00100000</td>
<td>→ 00100000</td>
</tr>
<tr>
<td>00010000</td>
<td>→ 00010000</td>
</tr>
<tr>
<td>00001000</td>
<td>→ 00001000</td>
</tr>
<tr>
<td>00000100</td>
<td>→ 00000100</td>
</tr>
<tr>
<td>00000010</td>
<td>→ 00000010</td>
</tr>
<tr>
<td>00000001</td>
<td>→ 00000001</td>
</tr>
</tbody>
</table>

Can this be learned?
Neural networks for data compression

Learned hidden layer representation:

<table>
<thead>
<tr>
<th>Input</th>
<th>Hidden Values</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>100000000</td>
<td>→ .89 .04 .08</td>
<td>→ 10000000</td>
</tr>
<tr>
<td>010000000</td>
<td>→ .01 .11 .88</td>
<td>→ 01000000</td>
</tr>
<tr>
<td>001000000</td>
<td>→ .01 .97 .27</td>
<td>→ 00100000</td>
</tr>
<tr>
<td>000100000</td>
<td>→ .99 .97 .71</td>
<td>→ 00010000</td>
</tr>
<tr>
<td>000010000</td>
<td>→ .03 .05 .02</td>
<td>→ 00001000</td>
</tr>
<tr>
<td>000001000</td>
<td>→ .22 .99 .99</td>
<td>→ 00000100</td>
</tr>
<tr>
<td>000000100</td>
<td>→ .80 .01 .98</td>
<td>→ 00000010</td>
</tr>
<tr>
<td>000000010</td>
<td>→ .60 .94 .01</td>
<td>→ 00000001</td>
</tr>
<tr>
<td>000000001</td>
<td>→ .60 .94 .01</td>
<td>→ 00000001</td>
</tr>
</tbody>
</table>
Training

Sum of squared errors for each output unit
Training

Hidden unit encoding for input 01000000
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
Overfitting in neural networks

- Robot perception task (example 1)
Overfitting in neural networks

- Robot perception task (example 2)
Avoiding overfitting in neural networks

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:

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

Weight sharing

Early stopping
Expressiveness of multilayer neural networks

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
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers
Expressiveness of multilayer neural networks

Figure 5.19. A two-layer, feed-forward neural network for the XOR problem.
Expressiveness of multilayer neural networks

- Trained two-layer network with three hidden units (\( \tanh \) activation function) and one linear output unit.
  - Blue dots: 50 data points from \( f(x) \), where \( x \) uniformly sampled over range \((-1, 1)\).
  - Grey dashed curves: outputs of the three hidden units.
  - Red curve: overall network function.

\[
f(x) = x^2
data points
\]

\[
f(x) = \sin(x)
\]

\[
f(\pi) = \sin(\pi)
\]
Expressiveness of multilayer neural networks

- Trained two-layer network with three hidden units (tanh activation function) and one linear output unit.
  - Blue dots: 50 data points from $f(x)$, where $x$ uniformly sampled over range (-1, 1).
  - Grey dashed curves: outputs of the three hidden units.
  - Red curve: overall network function.

\[ f(x) = \text{abs}(x) \]

\[ f(x) = H(x) \]

Heaviside step function
Expressiveness of multilayer neural networks

- Two-class classification problem with synthetic data.
- Trained two-layer network with two inputs, two hidden units (\texttt{tanh} activation function) and one logistic sigmoid output unit.

Blue lines: 
- \( z = 0.5 \) contours for hidden units

Red line: 
- \( y = 0.5 \) decision surface for overall network

Green line: 
- optimal decision boundary computed from distributions used to generate data