Introduction

- Networks typically consisting of input, hidden, and output layers.
- Commonly referred to as multilayer perceptrons.
- Popular learning algorithm is the error backpropagation algorithm (backpropagation, or backprop, for short), which is a generalization of the LMS rule.
  - Forward pass: activate the network, layer by layer
  - Backward pass: error signal backpropagates from output to hidden and hidden to input, based on which weights are updated.

Multilayer Perceptrons: Characteristics

- Each model neuron has a nonlinear activation function, typically a logistic function: $y_j = \frac{1}{1 + \exp(-v_j)}$.
- Network contains one or more hidden layers (layers that are not either an input or an output layer).
- Network exhibits a high degree of connectivity.

Multilayer Networks

- Differentiable threshold unit: sigmoid $\phi(v) = \frac{1}{1 + \exp(-v)}$. Interesting property: $\frac{d\phi(v)}{dv} = \phi(v)(1 - \phi(v))$.
- Output: $y = \phi(x^T w)$
- Other functions: $\tanh(v) = \frac{1 - \exp(-2v)}{1 + \exp(-2v)}$
Multilayer Networks and Backpropagation

- Nonlinear decision surfaces.

(a) One output (b) Two hidden, one output

- Another example: XOR

Error Gradient for a Sigmoid Unit

From the previous page:
\[
\frac{\partial E}{\partial w_i} = - \sum_k (d_k - y_k) \frac{\partial y_k}{\partial v_k} \frac{\partial v_k}{\partial w_i}
\]

But we know:
\[
\frac{\partial y_k}{\partial v_k} = \frac{\partial \phi(v_k)}{\partial v_k} = y_k(1 - y_k)
\]
\[
\frac{\partial v_k}{\partial w_i} = \frac{\partial (x_k^T w)}{\partial w_i} = x_{i,k}
\]

So:
\[
\frac{\partial E}{\partial w_i} = - \sum_k (d_k - y_k)y_k(1 - y_k)x_{i,k}
\]

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 \( j \)
   \[
   \delta_j \leftarrow y_j(1 - y_j)(d_j - y_j)
   \]
3. For each hidden unit \( h \)
   \[
   \delta_h \leftarrow y_h(1 - y_h) \sum_{j \in \text{outputs}} w_{j,h} \delta_j
   \]
4. Update each network weight \( w_{i,j} \)
   \[
   w_{j,i} \leftarrow w_{j,i} + \Delta w_{j,i}
   \]
   \[
   \Delta w_{j,i} = \eta \delta_j x_{i}
   \]

Note: \( w_{j,i} \) is the weight from \( i \) to \( j \) (i.e., \( w_{j,i} \rightarrow i \)).
The δ Term

- For output unit:
  \[ \delta_j \leftarrow y_j (1 - y_j) (d_j - y_j) \]

- For hidden unit:
  \[ \delta_h \leftarrow y_h (1 - y_h) \sum_{j \in \text{outputs}} w_{jh} \delta_j \]

- In sum, δ is the derivative times the error.
- Derivation to be presented later.

Derivation of ∆w

- Want to update weight as:
  \[ \Delta w_{ji} = -\eta \frac{\partial E}{\partial w_{ji}} , \]
  where error is defined as
  \[ E(w) \equiv \frac{1}{2} \sum_{j \in \text{outputs}} (d_j - y_j)^2 \]

- Given \( v_j = \sum_i w_{ji} x_i \),
  \[ \frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial v_j} \frac{\partial v_j}{\partial w_{ji}} \]

- Different formula for output and hidden.

Derivation of ∆w: Output Unit Weights

From the previous page,
\[ \frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial v_j} \frac{\partial v_j}{\partial w_{ji}} \]

- First, calculate \( \frac{\partial E}{\partial v_j} \):
  \[ \frac{\partial E}{\partial v_j} = \frac{\partial}{\partial v_j} \frac{\partial}{\partial y_j} y_j (1 - y_j) \]
  \[ = \frac{\partial}{\partial y_j} \frac{1}{2} (d_j - y_j)^2 \]
  \[ = \frac{\partial}{\partial y_j} \frac{1}{2} (d_j - y_j)^2 \]
  \[ = 2 \frac{1}{2} (d_j - y_j) \frac{\partial (d_j - y_j)}{\partial y_j} \]
  \[ = -(d_j - y_j) \frac{\partial y_j}{\partial v_j} \]
  \[ = -(d_j - y_j) \phi'(v_j) \]

Next, calculate \( \frac{\partial y_j}{\partial v_j} \):
\[ \phi'(v_j) = y_j (1 - y_j) \]
\[ \frac{\partial y_j}{\partial v_j} = y_j (1 - y_j) \]

Putting everything together,
\[ \frac{\partial E}{\partial v_j} = \frac{\partial E}{\partial y_j} \frac{\partial y_j}{\partial v_j} = -(d_j - y_j) y_j (1 - y_j) \]
Derivation of $\Delta w$: Output Unit Weights

From the previous page:

$$\frac{\partial E}{\partial v_j} = \frac{\partial E}{\partial y_j} \frac{\partial y_j}{\partial v_j} = -(d_j - y_j)y_j(1 - y_j).$$

Since

$$\frac{\partial v_j}{\partial w_{ji}} = \frac{\partial}{\partial w_{ji}} \sum_i w_{ji} x_i = x_i,$$

$$\frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial v_j} \frac{\partial v_j}{\partial w_{ji}} = - (d_j - y_j)y_j(1 - y_j) \delta_j,$$

where $\delta_j = \text{error} \times \phi'(\text{net})$ and $\phi'(\text{net})$ is the derivative of the activation function.

Derivation of $\Delta w$: Hidden Unit Weights

Finally, given

$$\frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial v_j} \frac{\partial v_j}{\partial w_{ji}} = \frac{\partial E}{\partial v_j} x_i,$$

and

$$\frac{\partial E}{\partial v_j} = \sum_{k \in \text{Downstream}(j)} -\delta_k w_{kj} y_j(1 - y_j),$$

$$\Delta w_{ji} = -\eta \frac{\partial E}{\partial w_{ji}} = \eta [y_j(1 - y_j) \delta_j \phi'(\text{net})] x_i,$$

$$\Delta w_{ji}(n) = \eta \delta_j(n) \cdot y_i(n).$$

Summary

$\Delta w_{ji}(n)$ = learning rate $\cdot$ local gradient $\cdot$ input signal

**Figure 4.5** Signal-flow graph of a part of the adjoint system pertaining to back-propagation of error signals.
### Extension to Different Network Topologies

- **Arbitrary number of layers:** for neurons in layer $m$:
  \[ \delta_r = y_r(1 - y_r) \sum_{s \in \text{layer } m+1} w_{sr} \delta_s. \]
- **Arbitrary acyclic graph:**
  \[ \delta_r = y_r(1 - y_r) \sum_{s \in \text{Downstream}(r)} w_{sr} \delta_s. \]

### Backpropagation: Properties

- 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 with different initial weights).
- Minimizes error over training examples:
  - Will it generalize well to subsequent examples?
- Training can take thousands of iterations → slow!
- Using the network after training is very fast.

### Learning Rate and Momentum

- Tradeoffs regarding learning rate:
  - Smaller learning rate: smoother trajectory but slower convergence
  - Larger learning rate: fast convergence, but can become unstable.
- Momentum can help overcome the issues above.
  \[ \Delta w_{ji}(n) = \eta \delta_j(n) y_i(n) + \alpha \Delta w_{ji}(n - 1). \]

The update rule can be written as:
\[ \Delta w_{ji}(n) = \eta \sum_{t=0}^{n} \alpha^{n-t} \delta_j(t) y_i(t) = -\eta \sum_{t=0}^{n} \alpha^{n-t} \frac{\partial E(t)}{\partial w_{ji}(t)}. \]

### Momentum (cont’d)

- The weight vector is the sum of an exponentially weighted time series.
- Behavior:
  - When successive $\frac{\partial E(t)}{\partial w_{ji}(t)}$ take the same sign:
    Weight update is accelerated (speed up downhill).
  - When successive $\frac{\partial E(t)}{\partial w_{ji}(t)}$ have different signs:
    Weight update is damped (stabilize oscillation).
Sequential (online) vs. Batch Training

- **Sequential mode:**
  - Update rule applied after each input-target presentation.
  - Order of presentation should be randomized.
  - Benefits: less storage, stochastic search through weight space helps avoid local minima.
  - Disadvantages: hard to establish theoretical convergence conditions.

- **Batch mode:**
  - Update rule applied after all input-target pairs are seen.
  - Benefits: accurate estimate of the gradient, convergence to local minimum is guaranteed under simpler conditions.

Representational Power of Feedforward Networks

- **Boolean functions:** every boolean function representable with two layers (hidden unit size can grow exponentially in the worst case: one hidden unit per input example, and “OR” them).
- **Continuous functions:** every bounded continuous function can be approximated with an arbitrarily small error (output units are linear).
- **Arbitrary functions:** with three layers (output units are linear).

What the Hidden Layer Does

- A smooth ramped output, monotonically increasing.
- Ramp can be oriented in different angles.
- This kind of visualization is only possible with low-dimensional input.

What the Hidden Layer Does (cont’d)

- We can also look at the hidden layer weight as a pattern or feature.
- Or, we can activate one hidden unit and see what output pattern it produces (example above).
Learned Hidden Layer Representations

Inputs Outputs

<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>
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<td>00000010</td>
<td>00000010</td>
</tr>
<tr>
<td>00000001</td>
<td>00000001</td>
</tr>
</tbody>
</table>

Learned Hidden Layer Representations

- Learned encoding is similar to standard 3-bit binary code.
- Automatic discovery of useful hidden layer representations is a key feature of ANN.
- Note: The hidden layer representation is compressed.

Overfitting

- Error in two different robot perception tasks.
- Training set and validation set error.
- Early stopping ensures good performance on unobserved samples, but must be careful.
- Weight decay, use of validation sets, use of \( k \)-fold cross-validation, etc. to overcome the problem.
Recurrent Networks

- Sequence recognition.
- Store tree structure (next slide).
- Can be trained with plain backpropagation.
- Generalization may not be perfect.

Some Applications: NETtalk

- Learn to pronounce English text.
- Demo
- Data available in UCI ML repository

NETtalk data

- aardvark a-rdvark 1<<<02<<0
- aback xb@k-0>1<<0
- abacus @bxkxs 1<0>0<0
- abaft xb@ft 0>1<<0
- abalone @bxloni 2<0>1>00
- abandon xb@ndxnx 0>1<<0
- abase xbes-0>1<<0
- abash xb@S-0>1<<0
- abate xbet-0>1<<0
- abatis @bxi-1<0>2<2
  ...

- Word – Pronunciation – Stress/Syllable
- about 20,000 words
More Applications: Data Compression

- Construct an autoassociative memory where Input = Output.
- Train with small hidden layer.
- Encode using input-to-hidden weights.
- Send or store hidden layer activation.
- Decode received or stored hidden layer activation with the hidden-to-output weights.

Backpropagation Exercise

- **URL:** [http://www.cs.tamu.edu/faculty/choe/src/backprop-1.6.tar.gz](http://www.cs.tamu.edu/faculty/choe/src/backprop-1.6.tar.gz)
- Untar and read the README file:
  
  ```
  gzip -dc backprop-1.6.tar.gz | tar xvf -
  ```
- Run `make` to build (on departmental unix machines).
- Run `./bp conf/xor.conf` etc.

Backpropagation: Example Results

- Epoch: one full cycle of training through all training input patterns.
- **OR** was easiest, **AND** the next, and **XOR** was the most difficult to learn.
- Network had 2 input, 2 hidden and 1 output unit. Learning rate was 0.001.

Backpropagation: Example Results (cont’d)

Output to (0,0), (0,1), (1,0), and (1,1) form each row.
Backpropagation: Things to Try

- How does increasing the number of hidden layer units affect the (1) time and the (2) number of epochs of training?
- How does increasing or decreasing the learning rate affect the rate of convergence?
- How does changing the slope of the sigmoid affect the rate of convergence?
- Different problem domains: handwriting recognition, etc.

MLP as a General Function Approximator

- MLP can be seen as performing **nonlinear input-output mapping**.
- **Universal approximation theorem**: Let $\phi(\cdot)$ be a nonconstant, bounded, monotone-increasing continuous function. Let $I_{m_0}$ denote the $m_0$-dimensional unit hypercube $[0, 1]^{m_0}$. The space of continuous functions on $I_{m_0}$ is denoted by $C(I_{m_0})$. Then given any function $f \in C(I_{m_0})$ and $\epsilon > 0$, there exists an integer $m_1$ and a set of real constants $\alpha_i, b_i,$ and $w_{ij}$, where $i = 1, \ldots, m_1$ and $j = 1, \ldots, m_0$, such that we may define

$$F(x_1, \ldots, x_{m_0}) = \sum_{i=1}^{m_1} \alpha_i \phi \left( \sum_{j=1}^{m_0} w_{ij} x_j + b_i \right)$$

as an approximate realization of the function $f(\cdot)$; that is

$$|F(x_1, \ldots, x_{m_0}) - f(x_1, \ldots, x_{m_0})| < \epsilon$$

for all $x_1, \ldots, x_{m_0}$ that lie in the input space.

MLP as a General Function Approximator (cont’d)

- The universal approximation theorem is an existence theorem, and it merely generalizes approximations by finite Fourier series.
- The universal approximation theorem is directly applicable to neural networks (MLP), and it implies that one hidden layer is sufficient.
- The theorem does not say that a single hidden layer is optimum in terms of learning time, generalization, etc.

Generalization

- A network is said to **generalize** well when the input-output mapping computed by the network is correct (or nearly so) for test data never used during training.
- This view is apt when we take the **curve-fitting view**.
- Issues: **overfitting** or **overtraining**, due to memorization. **Smoothness** in the mapping is desired, and this is related to criteria like Occam’s razor.
Generalization and Training Set Size

- Generalization is influenced by three factors:
  - Size of the training set, and how representative they are.
  - The architecture of the network.
  - Physical complexity of the problem.

- Sample complexity and VC dimension are related. In practice,

\[ N = O\left(\frac{W}{\epsilon}\right) \]

where \( W \) is the total number of free parameters, and \( \epsilon \) is the error tolerance.

Training Set Size and Curse of Dimensionality

- As the dimensionality of the input grows, exponentially more inputs are needed to maintain the same density in unit space.

- In other words, the sampling density of \( N \) inputs in \( m \)-dimensional space is proportional to \( N^{1/m} \).

- One way to overcome this is to use prior knowledge about the function.

Cross-Validation

- Use of validation set (not used during training, used for measuring generalizability).

  - Model selection
  - Early stopping
  - Hold-out method: multiple cross-validation, leave-one-out method, etc.

Virtues and Limitations of Backprop

- Connectionism: biological metaphor, local computation, graceful degradation, parallellism. (Some limitations exist regarding the biological plausibility of backprop.)

- Feature detection: hidden neurons perform feature detection.

- Function approximation: a form of nested sigmoid.

- Computational complexity: computation is polynomial in the number of adjustable parameters, thus it can be said to be efficient.

- Sensitivity analysis: sensitivity \( S_{\omega} = \frac{\partial F/\partial \omega}{\partial \omega} \) can be estimated efficiently.

- Robustness: disturbances can only cause small estimation errors.

- Convergence: stochastic approximation, and it can be slow.

- Local minima and scaling issues
Heuristic for Accelerating Convergence

Learning rate adaptation

- Separate learning rate for each tunable weight.
- Each learning rate is allowed to adjust after each iteration.
- If the derivative of the cost function has the same sign for several iterations, increase the learning rate.
- If the derivative of the cost function alternates the sign over several iterations, decrease the learning rate.

Summary

- Backprop for MLP is **local** and **efficient** (in calculating the partial derivative).
- Backprop can handle **nonlinear** mappings.