An Introduction to Neural Networks

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Neural Networks

Outline

Fundamentals

- Classes
- Design and Verification
- Results and Discussion
- Conclusion





Neural Networks

What Are They Used For?

Classification

- Pattern recognition, feature extraction, image matching
- Noise Reduction
 - Recognize patterns in the inputs and produce noiseless outputs
- Prediction

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Extrapolation based on historical data

Why Use Neural Networks?

Ability to learn

- NN's figure out how to perform their function on their own
- Determine their function based only upon sample inputs

Ability to generalize

i.e. produce reasonable outputs for inputs it has not been taught how to deal with

How Do Neural Networks Work?

Fundamentals

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The output of a neuron is a function of the weighted sum of the inputs plus a bias



 The function of the entire neural network is simply the computation of the outputs of all the neurons

An entirely deterministic calculation

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Activation Functions

- Applied to the weighted sum of the inputs of a neuron to produce the output
- Majority of NN's use sigmoid functions
 - Smooth, continuous, and monotonically increasing (derivative is always positive)
 - Bounded range but never reaches max or min
 - Consider "ON" to be slightly less than the max and "OFF" to be slightly greater than the min



Activation Functions

- The most common sigmoid function used is the logistic function
 - ► $f(x) = 1/(1 + e^{-x})$
 - The calculation of derivatives are important for neural networks and the logistic function has a very nice derivative
 - f'(x) = f(x)(1 f(x))
- Other sigmoid functions also used
 - hyperbolic tangent
 - arctangent
- The exact nature of the function has little effect on the abilities of the neural network

Where Do The Weights Come From?

- The weights in a neural network are the most important factor in determining its function
- Training is the act of presenting the network with some sample data and modifying the weights to better approximate the desired function
 - There are two main types of training
 - Supervised Training
 - Supplies the neural network with inputs and the desired outputs
 - Response of the network to the inputs is measured
 - The weights are modified to reduce the difference between the actual and desired outputs

Where Do The Weights Come From?

- Unsupervised Training
 - Only supplies inputs
 - The neural network adjusts its own weights so that similar inputs cause similar outputs
 - The network identifies the patterns and differences in the inputs without any external assistance

Epoch

- One iteration through the process of providing the network with an input and updating the network's weights
- Typically many epochs are required to train the neural network

Perceptrons First neural network with the ability to learn Classes Made up of only input neurons and output neurons Input neurons typically have two states: ON and OFF Output neurons use a simple threshold activation function In basic form, can only solve linear problems Limited applications .5 .2 Input Neurons Weights **Output Neuron**

Neural Networks



Classes

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Multilayer Feedforward Networks

- Most common neural network
- An extension of the perceptron
 - Multiple layers
 - The addition of one or more "hidden" layers in between the input and output layers
 - Activation function is not simply a threshold
 - Usually a sigmoid function
 - A general function approximator
 - Not limited to linear problems
- Information flows in one direction
 - The outputs of one layer act as inputs to the next layer





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Most common measure of error is the mean

 $E = (target - output)^2$

Partial derivatives of the error wrt the weights:

Output Neurons:

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let: \delta_j = f'(net_j) (target_j - output_j)
\partial E / \partial w_{ii} = -output_i \delta_i
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j = output neuron i = neuron in last hidden

Hidden Neurons:

let: $\delta_j = f'(net_j) \Sigma(\delta_k w_{kj})$ $\partial E/\partial w_{ji} = -output_i \delta_j$

j = hidden neuron i = neuron in previous layer k = neuron in next layer

- Calculation of the derivatives flows backwards through the network, hence the name, backpropagation
 - These derivatives point in the direction of the maximum increase of the error function
- A small step (learning rate) in the opposite direction will result in the maximum decrease of the (local) error function:

 $w_{new} = w_{old} - \alpha \ \partial E / \partial w_{old}$

where α is the learning rate

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Backpropagation

The learning rate is important

- Too small
 - Convergence extremely slow
- Too large
 - May not converge

Momentum

- Tends to aid convergence
- Applies smoothed averaging to the change in weights:
 - $\Delta_{\text{new}} = \beta \Delta_{\text{old}} \alpha \ \partial E / \partial w_{\text{old}}$

 $w_{new} = w_{old} + \Delta_{new}$

- β is the momentum coefficient
- Acts as a low-pass filter by reducing rapid fluctuations

Local Minima

- Training is essentially minimizing the mean square error function
 - Key problem is avoiding local minima
 - Traditional techniques for avoiding local minima:
 - Simulated annealing
 - ^a Perturb the weights in progressively smaller amounts
 - Genetic algorithms
 - [¤] Use the weights as chromosomes
 - Apply natural selection, mating, and mutations to these chromosomes

Counterpropagation (CP) Networks

- Another multilayer feedforward network
- Up to 100 times faster than backpropagation
- Not as general as backpropagation
- Made up of three layers:

Classes



How Do They Work?

• Kohonen Layer:

- Neurons in the Kohonen layer sum all of the weighted inputs received
- The neuron with the largest sum outputs a 1 and the other neurons output 0
- Grossberg Layer:
 - Each Grossberg neuron merely outputs the weight of the connection between itself and the one active Kohonen neuron

Why Two Different Types of Layers?

- More accurate representation of biological neural networks
- Each layer has its own distinct purpose:
 - Kohonen layer separates inputs into separate classes
 - Inputs in the same class will turn on the same Kohonen neuron
 - Grossberg layer adjusts weights to obtain acceptable outputs for each class

Classes

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Training a CP Network

Training the Kohonen layer

- Uses unsupervised training
- Input vectors are often normalized

The one active Kohonen neuron updates its weights according to the formula:

 $w_{new} = w_{old} + \alpha(input - w_{old})$ where α is the learning rate

- The weights of the connections are being modified to more closely match the values of the inputs
- At the end of training, the weights will approximate the average value of the inputs in that class



Hidden Layers and Neurons

- For most problems, one layer is sufficient
- Two layers are required when the function is discontinuous
- The number of neurons is very important:
 - ► Too few
 - Underfit the data NN can't learn the details
 - Too many
 - Overfit the data NN learns the insignificant details
 - Start small and increase the number until satisfactory results are obtained



How is the Training Set Chosen?

- Overfitting can also occur if a "good" training set is not chosen
- What constitutes a "good" training set?
 - Samples must represent the general population
 - Samples must contain members of each class
 - Samples in each class must contain a wide range of variations or noise effect

Size of the Training Set

- The size of the training set is related to the number of hidden neurons
 - Eg. 10 inputs, 5 hidden neurons, 2 outputs:
 - 11(5) + 6(2) = 67 weights (variables)
 - If only 10 training samples are used to determine these weights, the network will end up being overfit
 - Any solution found will be specific to the 10 training samples
 - Analogous to having 10 equations, 67 unknowns à you can come up with a specific solution, but you can't find the general solution with the given information

Training and Verification

- The set of all known samples is broken into two orthogonal (independent) sets:
 - Training set
 - A group of samples used to train the neural network
 - Testing set
 - A group of samples used to test the performance of the neural network
 - Used to estimate the error rate



Design

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Verification

- Provides an unbiased test of the quality of the network
- Common error is to "test" the neural network using the same samples that were used to train the neural network
 - The network was optimized on these samples, and will obviously perform well on them
 - Doesn't give any indication as to how well the network will be able to classify inputs that weren't in the training set

Verification

- Various metrics can be used to grade the performance of the neural network based upon the results of the testing set
 - Mean square error, SNR, etc.
- Resampling is an alternative method of estimating error rate of the neural network
 - Basic idea is to iterate the training and testing procedures multiple times
 - Two main techniques are used:
 - Cross-Validation
 - Bootstrapping



Results

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 A number of toy problems were tested on multilayer feedforward NN's with a single hidden layer and backpropagation:

Inverter

- The NN was trained to simply output 0.1 when given a "1" and 0.9 when given a "0"
 - A demonstration of the NN's ability to memorize
- 1 input, 1 hidden neuron, 1 output
- With learning rate of 0.5 and no momentum, it took about 3,500 epochs for sufficient training
- Including a momentum coefficient of 0.9 reduced the number of epochs required to about 250

- Inverter (continued)
 - Increasing the learning rate decreased the training time without hampering convergence for this simple example
 - Increasing the epoch size, the number of samples per epoch, decreased the number of epochs required and seemed to aid in convergence (reduced fluctuations)
 - Increasing the number of hidden neurons decreased the number of epochs required
 - Allowed the NN to better memorize the training set the goal of this toy problem
 - Not recommended to use in "real" problems, since the NN loses its ability to generalize

AND gate

- 2 inputs, 2 hidden neurons, 1 output
- About 2,500 epochs were required when using momentum

XOR gate

- Same as AND gate
- 3-to-8 decoder
 - 3 inputs, 3 hidden neurons, 8 outputs
 - About 5,000 epochs were required when using momentum

Absolute sine function approximator (|sin(x)|)

- A demonstration of the NN's ability to learn the desired function, |sin(x)|, and to generalize
- 1 input, 5 hidden neurons, 1 output
- The NN was trained with samples between $-\pi/2$ and $\pi/2$
 - The inputs were rounded to one decimal place
 - The desired targets were scaled to between 0.1 and 0.9
- The test data contained samples in between the training samples (i.e. more than 1 decimal place)
 - The outputs were translated back to between 0 and 1
- About 50,000 epochs required with momentum
- Not smooth function at 0 (only piece-wise continuous)

Results and Discussion Gaussian function approximator (e^{-x²}) 1 input, 2 hidden neurons, 1 output Similar to the absolute sine function approximator, except that the domain was changed to between -3 and 3 About 10,000 epochs were required with momentum Smooth function

- Primality tester
 - **7** inputs, 8 hidden neurons, 1 output
 - The input to the NN was a binary number
 - The NN was trained to output 0.9 if the number was prime and 0.1 if the number was composite
 - Classification and memorization test
 - The inputs were restricted to between 0 and 100
 - About 50,000 epochs required for the NN to memorize the classifications for the training set
 - No attempts at generalization were made due to the complexity of the pattern of prime numbers
 - Some issues with local minima

Results and Discussion

- Prime number generator
 - Provide the network with a seed, and a prime number of the same order should be returned
 - 7 inputs, 4 hidden neurons, 7 outputs
 - Both the input and outputs were binary numbers
 - The network was trained as an autoassociative network
 - Prime numbers from 0 to 100 were presented to the network and it was requested that the network echo the prime numbers
 - The intent was to have the network output the closest prime number when given a composite number
 - After one million epochs, the network was successfully able to produce prime numbers for about 85 - 90% of the numbers between 0 and 100
 - Using Gray code instead of binary did not improve results
 - Perhaps needs a second hidden layer, or implement some heuristics to reduce local minima issues

Conclusion

- The toy examples confirmed the basic operation of neural networks and also demonstrated their ability to learn the desired function and generalize when needed
- The ability of neural networks to learn and generalize in addition to their wide range of applicability makes them very powerful tools

Questions and Comments



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