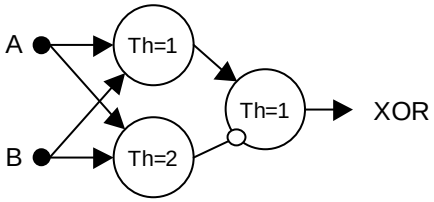
Lecture 11: Multi-layer perceptrons I

- **History of neural networks**
- **The back propagation algorithm**
- **Enhancements to steepest descent**
  - Momentum
  - Adaptive learning rates
  - Miscellaneous

A brief history of artificial neural networks (1)

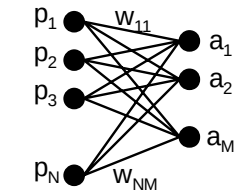
McCulloch and Pitts, 1943

- The modern era of neural networks starts in the 1940's, when Warren McCulloch (a psychiatrist and neuroanatomist) and Walter Pitts (a mathematician) explored the computational capabilities of networks made of very simple neurons
  - A McCulloch-Pitts network fires if the sum of its excitatory inputs exceeds its threshold, as long as it does not receive an inhibitory input
  - Using a network of such neurons, they showed that it was possible to construct any logical function



Hebb, 1949

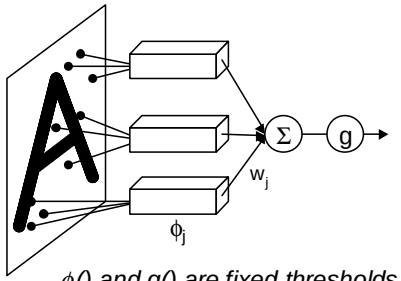
- In his book "The organization of Behavior", Donald Hebb introduced his postulate of learning (a.k.a. Hebbian learning), which states that the effectiveness of a variable synapse between two neurons is increased by the repeated activation of one neuron by the other across that synapse
  - The Hebbian rule has a strong similarity to the biological process in which a neural pathway is strengthened each time it is used



$$w_{ij}^{new} = + w_{ij}^{old} + \alpha\, p_i a_j$$

Rosenblatt, 1958

- Frank Rosenblatt introduced the perceptron, the simplest form of a neural network
  - The perceptron consists of a single neuron with adjustable synaptic weights and a threshold activation function
  - Rosenblatt's original perceptron in fact consisted of three layers (sensory, association and response) of with only only one layer had variable weights. As far as the variable weights are concerned, his original perceptron is similar to a single neuron
- Rosenblatt also developed an error-correction rule to adapt these weights (a.k.a. the perceptron learning rule), and proved that if the (two) classes were linearly separable, the algorithm would converge to a solution (a.k.a. the perceptron convergence theorem)



$\phi_j()$ and g() are fixed thresholds
w_j are variable weights

A brief history of artificial neural networks (2)

- **Widrow and Hoff, 1960**
  - At about the same time, Bernard Widrow and Ted Hoff introduced the Least-Mean-Square algorithm (a.k.a. delta-rule or Widrow-Hoff rule) and used it to train the Adaline (ADAptive Linear Neuron)
    - The Adaline was similar to the perceptron, except that it used a linear activation function instead of the threshold
    - The LMS algorithm is still heavily used in adaptive signal processing
- **Minsky and Papert, 1969**
  - During the 1950s and 1960s two school of thought: Artificial Intelligence and Connectionism, competed for prestige and funding
    - The AI community was interested in the highest cognitive processes: logic, rational though and problem solving
    - The Connectionists' principal model was the perceptron
      - The perceptron was severely limited in that it could only learn linearly separable patterns
      - Connectionists struggled to find a learning algorithm for multi-layer perceptrons that would not appear until the mid 1980s
  - In their monograph "Perceptrons", Marvin Minsky and Seymour Papert mathematically proved the limitations of Rosenblatt's perceptron and conjectured that multi-layered perceptrons would suffer from the same limitations

> The perceptron has shown itself worthy of study despite (and even because of!) its severe limitations. It has many features to attract attention: its linearity; its intriguing learning theorem; its clear paradigmatic simplicity as a kind of parallel computation. There is no reason to suppose that any of these virtues carry over to the many-layered version. Nevertheless, we consider it to be an important research problem to elucidate (or reject) our intuitive judgement that the extension to multilayer systems is sterile.
>
> M. Minsky and S. Papert, 1969

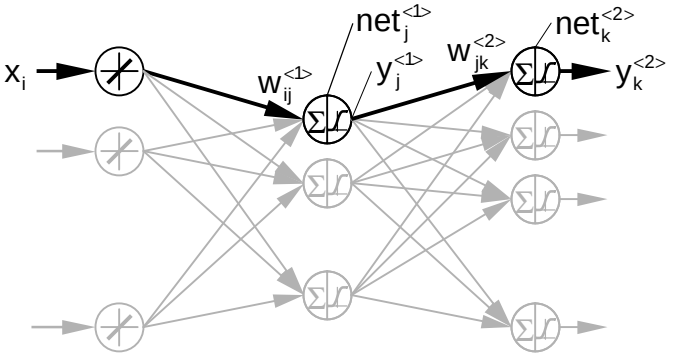
  - As a result of this monograph, research in neural networks was almost abandoned in the 1970s
  - Only a handful of researchers continued working on neural networks, mostly outside the United States
    - The 1970s saw the emergence of self-organizing maps [van der Malsburg, 1973], [Amari, 1977], [Grossberg, 1976] and associative memories: [Kohonen, 1972], [Anderson, 1972]

A brief history of artificial neural networks (3)

- **The resurgence of the early 1980s**
  - 1980: Grossberg (one of the few researchers in the United States that persevered despite the lack of support) establishes a new principle of self-organization called Adaptive Resonance Theory (ART) in collaboration with Carpenter
  - **1982: Hopfield explains the operation of a certain class of recurrent networks as an associative memory using statistical mechanics. These associative memories have come to be known as Hopfield networks. Along with backprop, Hopfield's work was most responsible for the rebirth of neural networks**
  - 1982: Kohonen presents self-organizing maps using one- and two-dimensional lattice structures. Kohonen SOMs have received far more attention than van der Malsburg's work and have become the benchmark for innovations in self-organization
  - 1983: Kirkpatrick, Gelatt and Vecchi introduced Simulated Annealing for solving combinatorial optimization problems. The concept of Simulated Annealing was later used by Ackley, Hinton and Sejnowsky (1985) to develop the Boltzmann machine (the first successful realization of multi-layered neural network)
  - 1983: Barto, Sutton and Anderson popularized reinforcement learning (it had been considered by Minsky in his 1954 PhD dissertation)
  - 1984: Braitenberg publishes his book "Vehicles" in which he advocates for a bottom-up approach to understand complex systems: start with very elementary mechanism and build up
- **Rumelhart, Hinton and Williams, 1986**
  - In 1986, Rumelhart, Hinton and Williams announced the discovery of a method that allowed a network to learn to discriminate between not linearly separable classes. They called the method "backward propagation of errors", a generalization of the LMS.
    - Backprop provided the solution to the problem that had puzzled Connectionists for two decades
    - Backprop was in reality a multiple invention: David Parker (1982, 1985) and Yann LeCun (1986) published similar discoveries
    - However, the honor of discovering backprop goes to **Paul Werbos** who presented these techniques in his 1974 Ph.D. dissertation at Harvard University

The back propagation algorithm (1)

- **Notation**
  - x_i is the i^{th} input to the network
  - $w_{ij}^{<1>}$ is the weight connecting the i^{th} input to the j^{th} hidden neuron
  - $net_j^{<1>}$ is the dot product at the j^{th} hidden neuron
  - $y_j^{<1>}$ is the output of the j^{th} hidden neuron
  - $w_{jk}^{<2>}$ is the weight connecting the k^{th} hidden neuron to the j^{th} output
  - $net_k^{<2>}$ is the dot product at the k^{th} output neuron
  - $y_k^{<2>}$ is the output of the k^{th} output neuron
  - t_k is the target (desired) output at the k^{th} output neuron
  - For simplicity we consider biases as regular weights with an input of 1



- **The goal of the MLP is to produce the desired target t_k at the k^{th} output for every pattern**
  - We will use the sum of squared errors at the output neurons as our objective function

$$J(W) = \sum_{n=1}^{N_{EX}} \sum_{k=1}^{N_O} \frac{1}{2} \left(t_k^{(n} - y_k^{<2>(n} \right)^2$$

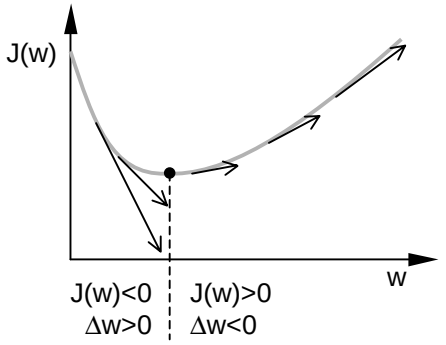
    - $t_k^{(n}$ is the desired target of the k^{th} output neuron for the n^{th} example
    - $y_k^{<2>(n}$ is the output of the k^{th} output neuron for the n^{th} example
  - For simplicity we will perform the derivation for one example (N_{EX}=1), allowing us to drop the outer summation

$$J(W) = \sum_{k=1}^{N_O} \frac{1}{2} \left(t_k - y_k^{<2>} \right)^2$$

    - W (upper case) denotes the set of all weights in the MLP
    - w (lower case) denotes a generic weight
  - Backprop performs steepest descent to update the weights after each iteration

$$w = w + \Delta w = w - \eta \frac{\partial J(W)}{\partial w}$$

    - The partial derivative $\partial J/\partial w$ indicates the direction of increasing values of J(w). Since we want to minimize J(w), we update the weights in the opposite direction to $\partial J/\partial w$



The back propagation algorithm (2)

- **The rest of this derivation is concerned with finding an expression of $\partial J/\partial w$ (for each weight) in terms of what we know: the inputs x_i, the outputs y_k and the targets t_k**
  - We will use the chain rule to express J(w) in terms of the weights and the perform the derivative
- **Calculation of $\partial J/\partial w$ for hidden-to output weights**
  - The output of the k^{th} output neuron (for a sigmoidal activation function) is

$$y_k^{<2>} = \frac{1}{1+\exp\left(-net_k^{<2>}\right)}$$

  - The dot product at the k^{th} output neuron is

$$net_k^{<2>} = \sum_{n=1}^{N_H} w_{nk}^{<2>} y_n^{<1>}$$

  - The derivative of J(W) with respect to a hidden-to-output weight is, using the chain rule

$$\frac{\partial J(W)}{\partial w_{jk}^{<2>}} = \frac{\partial J(W)}{\partial y_k^{<2>}} \frac{\partial y_k^{<2>}}{\partial net_k^{<2>}} \frac{\partial net_k^{<2>}}{\partial w_{jk}^{<2>}}$$

  - We calculate each of these terms separately

$$\frac{\partial J(W)}{\partial y_k^{<2>}} = \frac{\partial}{\partial y_k^{<2>}}\left[\sum_{n=1}^{N_O} \frac{1}{2}\left(y_n^{<2>} - t_n\right)^2\right] = \left(y_k^{<2>} - t_k\right)$$

$$\frac{\partial y_k^{<2>}}{\partial net_k^{<2>}} = \frac{\partial}{\partial net_k^{<2>}}\left[\frac{1}{1+\exp\left(-net_k^{<2>}\right)}\right] = \frac{\exp\left(-net_k^{<2>}\right)}{\left(1+\exp\left(-net_k^{<2>}\right)\right)^2} =$$

$$= \left[\frac{1+\exp\left(-net_k^{<2>}\right)-1}{1+\exp\left(-net_k^{<2>}\right)}\right]\left[\frac{1}{1+\exp\left(-net_k^{<2>}\right)}\right] = \left(1-y_k^{<2>}\right)y_k^{<2>}$$

$$\frac{\partial net_k^{<2>}}{\partial w_{jk}^{<2>}} = \frac{\partial}{\partial w_{jk}^{<2>}}\left[\sum_{n=1}^{N_H} w_{nk}^{<2>} y_n^{<1>}\right] = y_j^{<1>}$$

The back propagation algorithm (3)

- Merging all these derivatives yields

$$\frac{\partial J(W)}{\partial w_{jk}^{<2>}} = \left(y_k^{<2>} - t_k\right)\left(1 - y_k^{<2>}\right)y_k^{<2>}y_j^{<1>}$$

  - For the bias weights, use $y_j^{<1>}=1$ in the expression above

- **Calculation of $\partial J/\partial w$ for input-to-hidden weights**
  - The output of the j^{th} hidden neuron (for a sigmoidal activation function) is

$$y_j^{<1>} = \frac{1}{1+\exp\left(-net_j^{<1>}\right)}$$

  - The dot product at the j^{th} hidden neuron is

$$net_j^{<1>} = \sum_{n=1}^{N_I} w_{nj}^{<1>}x_n$$

  - The derivative of J(W) with respect to a input-to-hidden weight is, using the chain rule

$$\frac{\partial J(W)}{\partial w_{ij}^{<1>}} = \frac{\partial J(W)}{\partial y_j^{<1>}}\frac{\partial y_j^{<1>}}{\partial net_j^{<1>}}\frac{\partial net_j^{<1>}}{\partial w_{ij}^{<1>}}$$

  - The second and third terms are easy to calculate from our previous result

$$\frac{\partial y_j^{<1>}}{\partial net_j^{<1>}} = \left(1 - y_j^{<1>}\right)y_j^{<1>}$$

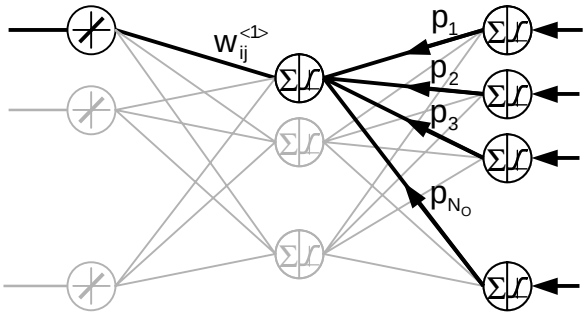
$$\frac{\partial net_j^{<1>}}{\partial w_{ij}^{<1>}} = x_i$$

  - The first term, however, is not straightforward since we do not know what the outputs of the hidden neurons ought to be
    - This is known as the **credit assignment problem** [Minski,1961], which puzzled connectionists for two decades

The back propagation algorithm (4)

- The trick to solve this puzzle is to realize that hidden neurons do not make errors but, rather, they contribute to the errors of the output nodes
  - The derivative of the network's error with respect to a hidden neuron's output is therefore the sum of that hidden node's contribution to the errors of all the output neurons

$$\frac{\partial J(W)}{\partial y_j^{<1>}} = \sum_{n=1}^{N_O} \frac{\partial J(W)}{\partial y_n^{<2>}} \frac{\partial y_n^{<2>}}{\partial net_n^{<2>}} \frac{\partial net_n^{<2>}}{\partial y_j^{<1>}}$$



- The first two terms in the summation are known from our earlier derivation

$$\frac{\partial J(W)}{\partial y_n^{<2>}} \frac{\partial y_n^{<2>}}{\partial net_n^{<2>}} = \left(y_n^{<2>} - t_n\right)\left(1 - y_n^{<2>}\right)y_n^{<2>} = p_n$$

- The last term in the summation is

$$\frac{\partial net_n^{<2>}}{\partial y_j^{<1>}} = w_{jn}^{<2>}$$

- Merging these derivatives yields

$$\frac{\partial J(W)}{\partial y_j^{<1>}} = \sum_{n=1}^{N_O} \frac{\partial J(W)}{\partial y_n^{<2>}} \frac{\partial y_n^{<2>}}{\partial net_n^{<2>}} \frac{\partial net_n^{<2>}}{\partial y_j^{<1>}} = \sum_{n=1}^{N_O} \underbrace{\left(y_n^{<2>} - t_n\right)\left(1 - y_n^{<2>}\right)y_n^{<2>}}_{p_n} w_{jn}^{<2>}$$

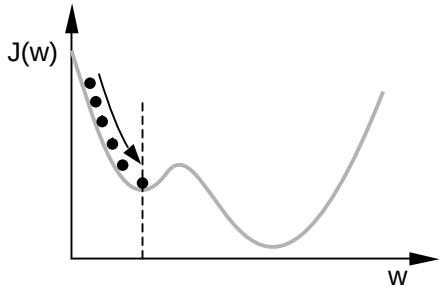
  - Notice that what we are actually doing is propagating the error term p_n backwards trough the hidden-to-output weighs (hence the term backprop)
- And the final expression of $\partial J/\partial w$ for input-to-hidden weights is

$$\frac{\partial J(W)}{\partial w_{ij}^{<1>}} = \left[\sum_{n=1}^{N_O} \left(y_n^{<2>} - t_n\right)\left(1 - y_n^{<2>}\right)y_n^{<2>} w_{jn}^{<2>}\right]\left(1 - y_j^{<1>}\right)y_j^{<1>} x_i$$

  - For the bias weights, use $x_i=1$ in the expression above

Enhancements to steepest descent: momentum

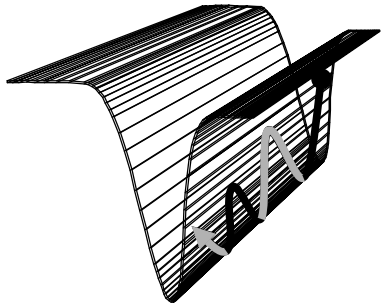
- **One of the main limitations of backprop is local minima**
  - When the steepest descent algorithm reaches a local minimum, the gradient becomes zero and the weights converge to a sub-optimal solution



- **A very popular method to overcome this limitation is to compute a temporal average of the direction in which the weights have been moving recently**
  - An easy way to implement this is by using an exponential average

$$\Delta w(n) = \mu[\Delta w(n-1)] + (1-\mu)\left[\eta \frac{\partial J(W)}{\partial w}\right]$$

  - The term μ is called the momentum and is a value between 0 and 1 (typically 0.9)
    - The closer to a value of 1, the stronger the influence of the instantaneous steepest descent direction



- **The momentum term is useful in spaces with long ravines characterized by sharp curvature across the ravine and a gently sloping floor**
  - Sharp curvature tends to cause divergent oscillations across the ravine
    - To avoid this problem, we could decrease the learning rate, but this is too slow
  - Momentum filters out the high curvature and allows the effective weight steps to be bigger
  - It turns out that ravines are not uncommon in optimization problems, so the use of momentum can be helpful in many situations
- **However, a momentum term can hurt when the search is close to the global minima (think of the error surface as a bowl)**
  - As the network approaches the bottom of the error surface, it builds enough momentum to propel the weights in the opposite direction, creating an undesirable oscillation that leads to slower convergence

More enhancements: adaptive learning rates

- **Rather than having a unique learning rate for all weights in the network, we can allow each weight to have its own learning rate and allow the learning rate to adapt based of the performance of the weight during training**
  - If the direction in which the objective function decreases w.r.t. a weight is the same as the direction in which it has been decreasing recently, make the learning rate larger. Otherwise decrease the learning rate.
- **The direction $\delta(n)$ in which the error decreases at time m is given by the sign of $\partial J/\partial w$**
- **The direction $\bar{\delta}(n)$ in which the error has been decreasing "recently" is computed as the exponential average of $\delta(n)$**

$$\bar{\delta}(n+1) = \theta\bar{\delta}(n) + [1-\theta]\delta(n)$$

  - θ is a parameter between 0 and 1 that controls how long "recently" means (typically 0.7)
- **To determine if the current direction and the recent direction coincide we multiply $\delta(n)$ by $\bar{\delta}(n)$**
  - If the product is greater than 0, the signs are the same
  - If the product is less than 0, the signs are the different
  - Based on this product we adapt the learning rates according to the following rule

$$\eta(n) = \begin{cases} \eta(n-1) + \kappa & \text{if } \bar{\delta}(n)\cdot\delta(n) > 0 \\ \eta(n-1)\psi & \text{if } \bar{\delta}(n)\cdot\delta(n) \le 0 \end{cases}$$

  - κ is a constant that is added to the learning rate if the direction has not changed (the actual value of κ is problem dependent)
  - Ψ is a fraction that is multiplied to the learning rate if the direction has changed (typically 0.5)
- **The final expression for the weight change, assuming also a momentum term, becomes**

$$\Delta w(n) = \mu[\Delta w(n-1)] + (1-\mu)\left[\eta(n)\frac{\partial J(W)}{\partial w}\right]$$

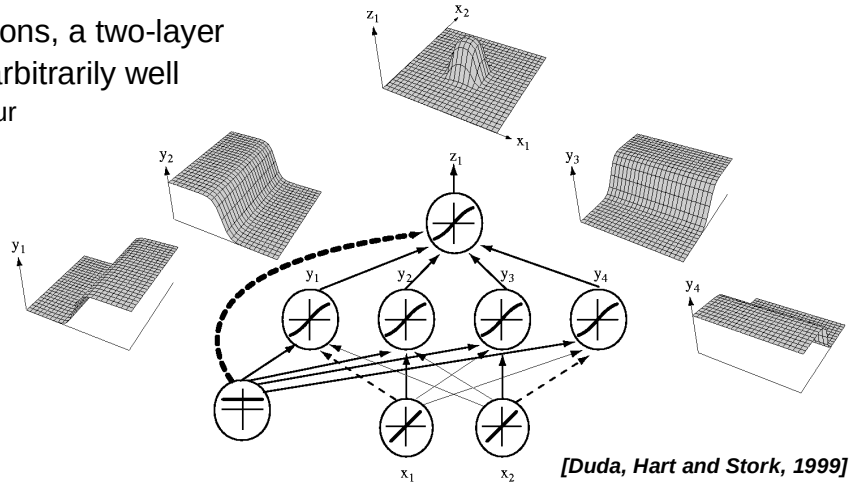
  - The adaptive nature of η is made explicit by making it a function of the iteration $\eta(n)$

Other techniques to improve backprop

- **Activation function**
  - A MLP trained with backprop will generally train faster if the activation function is anti-symmetric: f(-x)=-f(x)
    - The hyperbolic tangent function is the typical anti-symmetric function used in MLPs
- **Target values**
  - It is important that the target values are within the range of the activation function, otherwise the neuron will not be capable of matching the target value
  - In addition, it is recommended that the target values are not the limiting values of the activation function; otherwise backprop will tend to drive the neurons into saturation, slowing down the learning process
    - The slope of the activation function, which is proportional to Δw, becomes zero at $\pm\infty$
- **Input normalization**
  - Input variables should be preprocessed so that their mean value is zero or small compared to the variance
  - Input variables should be uncorrelated (use PCA to accomplish this)
  - Input variables should have the same variance (use Fukunaga's whitening transform)
- **Initial weights**
  - Initial random weights should be small to avoid driving the neurons into saturation
    - Hidden-to-output (HO) weights should be made larger than input-to-hidden (IH) weights since they carry the back propagated error. If the initial HO weights are very small, the weight changes at the IH layer will be initially very small, slowing the training procedure
- **Number of hidden neurons**
  - While the number of inputs and outputs are dictated by the problem, the number of hidden units is not related so directly to the application domain
  - The number of hidden units determines the degrees of freedom or expressive power of the model
    - A small number of hidden units may not be sufficient to model complex I/O mappings
    - A large number of hidden units may overfit the training data and prevent the network from generalizing to new examples
  - A good rule of thumb is to make the total number of weights in the network $1/10^{th}$ of the number of training examples

Other techniques to improve backprop

- **Weight decay**
  - To prevent the weights from growing too large (a sign of over-training) it is convenient to add a decay term of the form $\mathbf{w(n+1) = (1-\varepsilon)\bullet w(n)}$
    - Weights that are not needed eventually decay to zero, whereas necessary weights are continuously updated by backprop
- **Weight updates**
  - The derivation of backprop was based on one training example but, in practice, the data set contains a large number of examples
  - There are two basic approaches for updating the weights during training
    - On-line training: weights are updated after presentation of each example
    - Batch training: weights are updated after presentation of all the examples (we store the Δw for each example, and add them up the the weight after all the examples have been presented)
  - Batch training is recommended
    - Batch training uses the TRUE steepest descent direction
    - On-line training achieves lower errors earlier in training but only because the weights are updated n (# examples) times faster than in batch mode
    - On-line training is sensitive to the ordering of examples
- **Number of hidden layers**
  - Given a sufficiently large number of hidden neurons, a two-layer MLP can approximate any continuous function arbitrarily well
    - As an example, we show that a combination of four hidden neurons can produce a "bump" at the output space of a two-layered MLP
      - A large number of these "bumps" can approximate any surface arbitrarily well
  - However, In some applications it may be desirable to have multiple (>2) layers with different functionality
    - In other words, the "bump" analogy is simply a conceptual tool, it does not describe how MLPs actually work!!!



[Duda, Hart and Stork, 1999]