Hebbian Learning and Gradient Descent Learning

Neural Computation : Lecture 5

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Hebbian Learning

The neuropsychologist Donald Hebb postulated in 1949 how biological neurons learn:

> "When an axon of cell A is near enough to excite a cell B and repeatedly or persistently takes part in firing it, some growth process or metabolic change takes place on one or both cells such that A's efficiency as one of the cells firing B, is increased."

In more familiar terminology, that can be stated as the ***Hebbian Learning*** rule:

1. If two neurons on either side of a synapse (connection) are activated simultaneously (i.e. synchronously), then the strength of that synapse is selectively increased.

Then, in the notation used for Perceptrons, that can be written as the weight update:

$$\Delta w_{ij} = \eta . out_j . in_i$$

There is strong physiological evidence that this type of learning does take place in the region of the brain known as the *hippocampus*.

Modified Hebbian Learning

An obvious problem with the above rule is that it is unstable – chance coincidences will build up the connection strengths, and all the weights will tend to increase indefinitely. Consequently, the basic learning rule (1) is often supplemented by:

2. If two neurons on either side of a synapse are activated asynchronously, then that synapse is selectively weakened or eliminated.

Another way to stop the weights increasing indefinitely involves normalizing them so they are constrained to lie between 0 and 1. This is preserved by the weight update

$$\Delta w_{ij} = \frac{w_{ij} + \eta . out_j . in_i}{\left(\sum_k (w_{kj} + \eta . out_j . in_k)^2 \right)^{1/2}} - w_{ij}$$

which, using a small η and linear neuron approximation, leads to ***Oja's Learning Rule***

$$\Delta w_{ij} = \eta . out_j . in_i - \eta . out_j . w_{ij} . out_j$$

which is a useful stable form of Hebbian Learning.

Hebbian versus Perceptron Learning

It is instructive to compare the Hebbian and Oja learning rules with the ***Perceptron learning*** weight update rule we derived previously, namely:

$$\Delta w_{ij} = \eta.(targ_j - out_j).in_i$$

There is clearly some similarity, but the absence of the target outputs $targ_j$ means that Hebbian learning is never going to get a Perceptron to learn a set of training data.

There exist variations of Hebbian learning, such as ***Contrastive Hebbian Learning***, that do provide powerful supervised learning for biologically plausible networks.

However, it has been shown that, for many relevant cases, much simpler non-biologically plausible algorithms end up producing the same functionality as these biologically plausible Hebbian-type learning algorithms.

For the purposes of this module, we shall therefore pursue simpler non-Hebbian approaches for formulating learning algorithms for our artificial neural networks.

Learning by Error Minimisation

The general requirement for learning is an algorithm that adjusts the network weights w_{ij} to minimise the difference between the actual outputs out_j and the desired outputs $targ_j$.

It is natural to define an ***Error Function*** or ***Cost Function*** E to quantify this difference. There are many (problem dependent) possibilities, but one obvious example is

$$E_{SSE}(w_{ij}) = \tfrac{1}{2} \sum_p \sum_j \left(targ_j - out_j \right)^2$$

This is known as the ***Sum Squared Error*** (SSE) function – it is the total squared error summed over all the output units j and all the training patterns p. The process of training a neural network corresponds to minimizing such an error function.

We shall first look at the particularly simple special case of single layer regression networks, for which there is a simple direct computation that achieves the minimum, and then go on to look at the iterative procedures that are necessary for more complex networks, that have other structures, activation functions and error functions.

Single Layer Regression Networks

Regression or ***Function Approximation*** problems involve approximating an underlying function from a set of noisy data. In this case, the appropriate output activation function is normally the simple ***linear activation function*** $f(x) = x$, rather than some kind of step function as required for classification problems. This means the outputs of a single layer regression network take on the simple form:

$$out_j = \sum_{i=1}^{n} in_i w_{ij} - \theta_j = \sum_{i=0}^{n} in_i w_{ij}$$

Then, if we train the network by minimizing the Sum Squared Error on the outputs, the derivative of the error with respect to each weight must be zero at the minumum, i.e.

$$\frac{\partial}{\partial w_{kl}} \left[\tfrac{1}{2} \sum_p \sum_j \left(targ_j - \sum_i in_i w_{ij} \right)^2 \right] = 0$$

This is a set of simultaneous linear equations, one for each training pattern, and finding the weights in this case reduces to solving that set of equations for the w_{ij}.

Learning by Simple Matrix Inversion

If we introduce explicit training pattern labels p and compute the derivative we have

$$\sum_p \left(targ_{pl} - \sum_i in_{pi} w_{il} \right) in_{pk} = 0$$

and this set of equations can be written in conventional matrix form as

$$\mathbf{in}^{\mathsf{T}} \left(\mathbf{targ} - \mathbf{in}\ \mathbf{w} \right) = 0$$

which has a formal solution for the weights in terms of the input ***pseudo-inverse*** $\mathbf{in}^{\dagger}$

$$\mathbf{w} = \mathbf{in}^{\dagger}\ \mathbf{targ} = (\mathbf{in}^{\mathsf{T}}\ \mathbf{in})^{-1}\ \mathbf{in}^{\mathsf{T}}\ \mathbf{targ}$$

Thus, it is possible to compute the required network weights directly from the inputs and targets using standard matrix pseudo-inversion techniques.

Unfortunately, this simple matrix inversion approach will only work for this particularly simple case. In general, one has to use an iterative weight update procedure.

Gradient Descent Learning

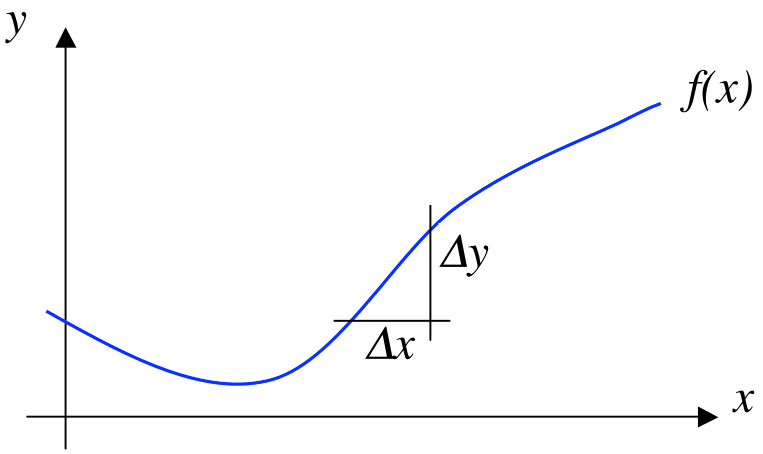
We have already seen how iterative weight updates work in Hebbian learning and the Perceptron Learning rule. The aim now is to develop a ***learning algorithm*** that minimises a cost function (such as Sum Squared Error) by making appropriate iterative adjustments to the weights w_{ij}. The idea is to apply a series of small updates to the weights $w_{ij} \rightarrow w_{ij} + \Delta w_{ij}$ until the cost $E(w_{ij})$ is "small enough".

For the Perceptron Learning Rule, we determined the direction that each weight needed to change to bring the output closer to the right side of the decision boundary, and then updated the weight by a small step in that direction.

Now we want to determine the direction that the ***weight vector*** needs to change to best reduce the chosen cost function. A systematic procedure for doing that requires knowledge of how the cost $E(w_{ij})$ varies as the weights w_{ij} change, i.e. the ***gradient*** of E with respect to w_{ij}. Then, if we repeatedly adjust the weights by small steps against the gradient, we will move through ***weight space***, descending along the gradients towards a minimum of the cost function.

Computing Gradients and Derivatives

The branch of mathematics concerned with computing gradients is called ***Differential Calculus***. The relevant general idea is straightforward. Consider a function $y = f(x)$:



The gradient of $f(x)$, at a particular value of x, is the rate of change of $f(x)$ as we change x, and that can be approximated by $\Delta y/\Delta x$ for small Δx. It can be written exactly as

$$\frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

which is known as the ***partial derivative*** of $f(x)$ with respect to x.

Examples of Computing Derivatives Analytically

Some simple examples illustrate how derivatives can be computed:

$$f(x) = a.x + b \qquad \Rightarrow \qquad \frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{[a.(x+\Delta x)+b]-[a.x+b]}{\Delta x} = a$$

$$f(x) = a.x^2 \qquad \Rightarrow \qquad \frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{\left[a.(x+\Delta x)^2\right]-\left[a.x^2\right]}{\Delta x} = 2ax$$

$$f(x) = g(x) + h(x) \quad \Rightarrow \quad \frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{\left(g(x+\Delta x)+h(x+\Delta x)\right)-\left(g(x)+h(x)\right)}{\Delta x} = \frac{\partial g(x)}{\partial x} + \frac{\partial h(x)}{\partial x}$$

Other derivatives can be found in the same way. Some particularly useful ones are:

$$f(x) = a.x^n \quad \Rightarrow \quad \frac{\partial f(x)}{\partial x} = nax^{n-1} \qquad\qquad f(x) = \log_e(x) \quad \Rightarrow \quad \frac{\partial f(x)}{\partial x} = \frac{1}{x}$$

$$f(x) = e^{ax} \quad \Rightarrow \quad \frac{\partial f(x)}{\partial x} = ae^{ax} \qquad\qquad f(x) = \sin(x) \quad \Rightarrow \quad \frac{\partial f(x)}{\partial x} = \cos(x)$$

Gradient Descent Minimisation

If we want to change the value of x to minimise a function $f(x)$, what we need to do depends on the gradient of $f(x)$ at the current value of x. There are three cases:

If $\frac{\partial f}{\partial x} > 0$ then $f(x)$ increases as x increases so we should decrease x

If $\frac{\partial f}{\partial x} < 0$ then $f(x)$ decreases as x increases so we should increase x

If $\frac{\partial f}{\partial x} = 0$ then $f(x)$ is at a maximum or minimum so we should not change x

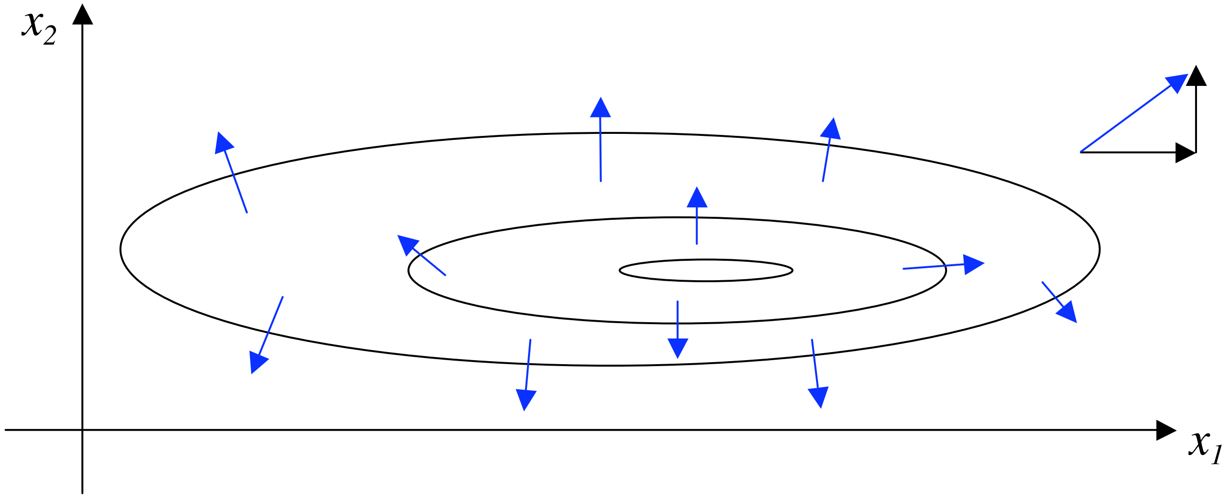
In summary, we can decrease $f(x)$ by changing x by the amount:

$$\Delta x = x_{new} - x_{old} = -\eta \frac{\partial f}{\partial x}$$

where η is a small positive constant specifying how much we change x by, and the derivative $\partial f/\partial x$ tells us which direction to go in. If we repeatedly use this equation, $f(x)$ will (assuming η is sufficiently small) keep descending towards a minimum, and hence this procedure is known as ***gradient descent minimisation***.

Gradients in More Than One Dimension

It might not be obvious that one needs the gradient/derivative itself in the weight update equation, rather than just the sign of the gradient. So, consider the two dimensional function shown as a ***contour plot*** with its minimum inside the smallest ellipse:



A few representative gradient vectors are shown. By definition, they will always be perpendicular to the contours, and the closer the contours, the larger the vectors. It is now clear that we need to take the relative magnitudes of the x_1 and x_2 components of the gradient vectors into account if we are to head towards the minimum efficiently.

Training a Single Layer Feed-forward Network

Now we know how gradient descent weight update rules can lead to minimisation of a neural network's output errors, it is straightforward to train any single layer network:

1. Take the set of training patterns you wish the network to learn

   $\{in_i^p, targ_j^p : i = 1 \ldots ninputs, j = 1 \ldots noutputs, p = 1 \ldots npatterns\}$
2. Set up the network with *ninputs* input units fully connected to *noutputs* output units via connections with weights w_{ij}
3. Generate random initial weights, e.g. from the range $[-smwt, +smwt]$
4. Select an appropriate error function $E(w_{ij})$ and learning rate η
5. Apply the weight update $\Delta w_{ij} = -\eta\, \partial E(w_{ij})/\partial w_{ij}$ to each weight w_{ij} for each training pattern p. One set of updates of all the weights for all the training patterns is called one ***epoch*** of training.
6. Repeat step 5 until the network error function is "small enough".

This will produce a trained neural network, but steps 4 and 5 can still be difficult…

Gradient Descent Error Minimisation

We will look at how to choose the error function E next lecture. Suppose, for now, that we want to train a single layer network by adjusting its weights w_{ij} to minimise the SSE:

$$E(w_{ij}) = \tfrac{1}{2}\sum_p \sum_j \left(targ_j - out_j\right)^2$$

We have seen that we can do this by making a series of gradient descent weight updates:

$$\Delta w_{kl} = -\eta \frac{\partial E(w_{ij})}{\partial w_{kl}}$$

If the transfer function for the output neurons is $f(x)$, and the activations of the previous layer of neurons are in_i, then the outputs are $out_j = f(\sum_i in_i w_{ij})$, and

$$\Delta w_{kl} = -\eta \frac{\partial}{\partial w_{kl}} \left[\tfrac{1}{2}\sum_p \sum_j \left(targ_j - f(\sum_i in_i w_{ij}) \right)^2 \right]$$

Dealing with equations like this is easy if we use the chain rules for derivatives.

Chain Rules for Computing Derivatives

Computing complex derivatives can be done in stages. First, suppose *f(x) = g(x).h(x)*

$$\frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{g(x+\Delta x).h(x+\Delta x) - g(x).h(x)}{\Delta x} = \lim_{\Delta x \to 0} \frac{\left(g(x) + \frac{\partial g(x)}{\partial x}\Delta x\right).\left(h(x) + \frac{\partial h(x)}{\partial x}\Delta x\right) - g(x).h(x)}{\Delta x}$$

$$\frac{\partial f(x)}{\partial x} = \frac{\partial g(x)}{\partial x} h(x) + g(x)\frac{\partial h(x)}{\partial x}$$

We can similarly deal with nested functions. Suppose *f(x) = g(h(x))*

$$\frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{g(h(x+\Delta x)) - g(h(x))}{\Delta x} = \lim_{\Delta x \to 0} \frac{g(h(x) + \frac{\partial h(x)}{\partial x}\Delta x) - g(h(x))}{\Delta x}$$

$$\frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{g(h(x)) + \frac{\partial g(x)}{\partial h(x)}\Delta h(x) - g(h(x))}{\Delta x} = \lim_{\Delta x \to 0} \frac{g(h(x)) + \frac{\partial g(x)}{\partial h(x)}\left(\frac{\partial h(x)}{\partial x}\Delta x\right) - g(h(x))}{\Delta x}$$

$$\frac{\partial f(x)}{\partial x} = \frac{\partial g(h(x))}{\partial h(x)} \cdot \frac{\partial h(x)}{\partial x}$$

Using the Chain Rule on the Weight Update Equation

The algebra gets rather messy, but after repeated application of the chain rule, and some tidying up, we end up with a very simple weight update equation:

$$\Delta w_{kl} = -\eta \frac{\partial}{\partial w_{kl}} \left[\tfrac{1}{2} \sum_p \sum_j \left(targ_j - f(\sum_i in_i w_{ij}) \right)^2 \right]$$

$$\Delta w_{kl} = -\eta \left[\tfrac{1}{2} \sum_p \sum_j \frac{\partial}{\partial w_{kl}} \left(targ_j - f(\sum_i in_i w_{ij}) \right)^2 \right]$$

$$\Delta w_{kl} = -\eta \left[\tfrac{1}{2} \sum_p \sum_j 2 \left(targ_j - f(\sum_i in_i w_{ij}) \right) \left(-\frac{\partial}{\partial w_{kl}} f(\sum_m in_m w_{mj}) \right) \right]$$

$$\Delta w_{kl} = \eta \left[\sum_p \sum_j \left(targ_j - f(\sum_i in_i w_{ij}) \right) \left(f'(\sum_n in_n w_{nj}) \frac{\partial}{\partial w_{kl}} (\sum_m in_m w_{mj}) \right) \right]$$

$$\Delta w_{kl} = \eta \left[\sum_{p} \sum_{j} \left(targ_{j} - f(\sum_{i} in_{i} w_{ij}) \right) \left(f'(\sum_{n} in_{n} w_{nj})(\sum_{m} in_{m} \frac{\partial w_{mj}}{\partial w_{kl}}) \right) \right]$$

$$\Delta w_{kl} = \eta \left[\sum_{p} \sum_{j} \left(targ_{j} - f(\sum_{i} in_{i} w_{ij}) \right) \left(f'(\sum_{n} in_{n} w_{ij})(\sum_{m} in_{m} \delta_{mk} \delta_{jl}) \right) \right]$$

$$\Delta w_{kl} = \eta \left[\sum_{p} \sum_{j} \left(targ_{j} - f(\sum_{i} in_{i} w_{ij}) \right) \left(f'(\sum_{n} in_{n} w_{nj})(in_{k} \delta_{jl}) \right) \right]$$

$$\Delta w_{kl} = \eta \left[\sum_{p} \left(targ_{l} - f(\sum_{i} in_{i} w_{il}) \right) \left(f'(\sum_{n} in_{n} w_{nl})(in_{k}) \right) \right]$$

$$\Delta w_{kl} = \eta \sum_{p} \left(targ_{l} - out_{l} \right) . f'(\sum_{n} in_{n} w_{nl}) . in_{k}$$

The *prime notation* is defined such that f' is the derivative of f. We have also used the *Kronecker Delta* symbol δ_{ij} defined such that $\delta_{ij} = 1$ when $i = j$ and $\delta_{ij} = 0$ when $i \neq j$.

The Delta Rule

We thus have the gradient descent learning algorithm for single layer SSE networks:

$$\Delta w_{kl} = \eta \sum_p \left(targ_l - out_l \right).f'\left(\sum_n in_n w_{nl} \right).in_k$$

Notice that these weight updates involve the derivative $f'(x)$, so the activation function $f(x)$ must be differentiable for gradient descent learning to work. This is clearly no good for simple classification Perceptrons which use the step function step(x) as their threshold function, because that has zero derivative everywhere except at $x = 0$ where it is infinite. We will need to use a smoothed version of a step function, like a sigmoid. However, for a linear activation function $f(x) = x$, appropriate for regression, we have weight updates

$$\Delta w_{kl} = \eta \sum_p \left(targ_l - out_l \right).in_k$$

which is often known as the ***Delta Rule*** because each update Δw_{kl} is simply proportional to the relevant input in_k and the corresponding output discrepancy $delta_l = targ_l - out_l$. This update rule is exactly the same as the Perceptron Learning Rule we derived earlier.

Delta Rule vs. Perceptron Learning Rule

We have seen that the Delta Rule and the Perceptron Learning Rule for training Single Layer Perceptrons have exactly the same weight update equation.

However, the two algorithms were obtained from very different theoretical starting points. The Perceptron Learning Rule was derived from a consideration of how we should shift around the decision hyper-planes for step function outputs, while the Delta Rule emerged from a gradient descent minimisation of the Sum Squared Error for a linear output activation function.

The Perceptron Learning Rule will converge to zero error and no weight changes in a finite number of steps if the problem is linearly separable, but otherwise the weights will keep oscillating. On the other hand, the Delta Rule will (for sufficiently small η) always converge to a set of weights for which the error is a minimum, though the convergence to the precise target values will generally proceed at an ever decreasing rate proportional to the output discrepancies $delta_l$.

Overview and Reading

1. We began with a brief look at Hebbian Learning and Oja's Rule.
2. We then considered how neural network weight learning could be put into the form of minimising an appropriate output error or cost function.
3. We looked at the special case of how simple matrix pseudo-inversion could be used to find the weights for single layer regression networks.
4. Then we saw how to compute the gradients/derivatives that enable us to formulate efficient general error minimisation algorithms, and how they can be used to derive the Delta Rule for training single layer networks.

Reading

1. Bishop: Sections 3.1, 3.2, 3.3, 3.4, 3.5
2. Haykin-1999: Sections 2.2, 2.4, 3.3, 3.4, 3.5
3. Gurney: Sections 5.1, 5.2, 5.3
4. Beale & Jackson: Section 4.4
5. Callan: Sections 2.1, 2.2